Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 03:23 PM EDT

PDB ID	:	1YJX
Title	:	Crystal structure of human B type phosphoglycerate mutase
Authors	:	Wang, Y.; Wei, Z.; Liu, L.; Gong, W.
Deposited on	:	2005-01-16
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

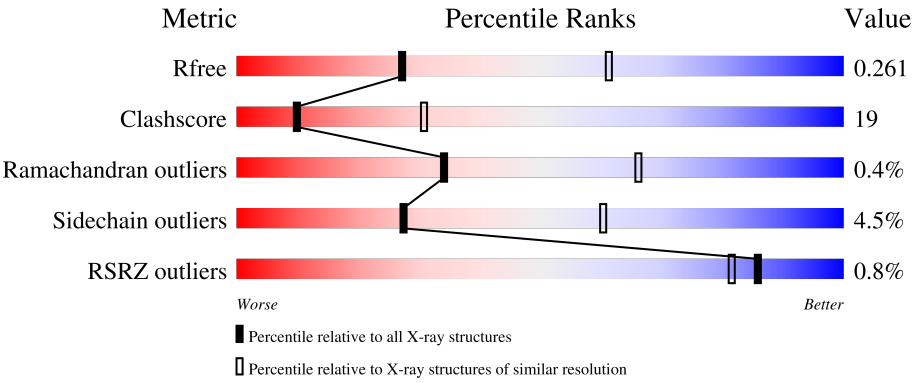
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	262	63% 27% 6%
1	B	262	63% 26% 8%
1	C	262	63% 28% 7%
1	D	262	64% 27% 6%
1	E	262	65% 27% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	262	62% 29% 8%
1	G	262	58% 32% 6%
1	H	262	56% 33% 8%
1	I	262	55% 35% 8%
1	J	262	58% 34% 7%
1	K	262	60% 30% 9%
1	L	262	61% 30% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CIT	B	602	-	X	-	-
3	CIT	C	603	-	X	-	-
3	CIT	D	604	-	X	-	-
3	CIT	E	605	-	X	-	-
3	CIT	F	606	-	X	-	-
3	CIT	H	608	-	X	-	-
3	CIT	I	609	-	X	-	-
3	CIT	J	610	-	X	-	-
3	CIT	K	611	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23286 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phosphoglycerate mutase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1913	1218	337	351	7			
1	B	242	Total	C	N	O	S	0	0	0
			1903	1211	335	350	7			
1	C	243	Total	C	N	O	S	0	0	0
			1898	1209	332	351	6			
1	D	245	Total	C	N	O	S	0	0	0
			1914	1218	336	353	7			
1	E	243	Total	C	N	O	S	0	0	0
			1897	1208	332	351	6			
1	F	242	Total	C	N	O	S	0	0	0
			1890	1204	332	347	7			
1	G	245	Total	C	N	O	S	0	0	0
			1887	1200	329	351	7			
1	H	241	Total	C	N	O	S	0	0	0
			1875	1196	328	345	6			
1	I	242	Total	C	N	O	S	0	0	0
			1904	1213	332	352	7			
1	J	244	Total	C	N	O	S	0	0	0
			1918	1220	339	352	7			
1	K	239	Total	C	N	O	S	0	0	0
			1870	1193	332	340	5			
1	L	245	Total	C	N	O	S	0	0	0
			1921	1222	342	350	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	LEU	-	expression tag	UNP P18669
A	256	GLU	-	expression tag	UNP P18669
A	257	HIS	-	expression tag	UNP P18669
A	258	HIS	-	expression tag	UNP P18669
A	259	HIS	-	expression tag	UNP P18669

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	HIS	-	expression tag	UNP P18669
A	261	HIS	-	expression tag	UNP P18669
A	262	HIS	-	expression tag	UNP P18669
B	255	LEU	-	expression tag	UNP P18669
B	256	GLU	-	expression tag	UNP P18669
B	257	HIS	-	expression tag	UNP P18669
B	258	HIS	-	expression tag	UNP P18669
B	259	HIS	-	expression tag	UNP P18669
B	260	HIS	-	expression tag	UNP P18669
B	261	HIS	-	expression tag	UNP P18669
B	262	HIS	-	expression tag	UNP P18669
C	255	LEU	-	expression tag	UNP P18669
C	256	GLU	-	expression tag	UNP P18669
C	257	HIS	-	expression tag	UNP P18669
C	258	HIS	-	expression tag	UNP P18669
C	259	HIS	-	expression tag	UNP P18669
C	260	HIS	-	expression tag	UNP P18669
C	261	HIS	-	expression tag	UNP P18669
C	262	HIS	-	expression tag	UNP P18669
D	255	LEU	-	expression tag	UNP P18669
D	256	GLU	-	expression tag	UNP P18669
D	257	HIS	-	expression tag	UNP P18669
D	258	HIS	-	expression tag	UNP P18669
D	259	HIS	-	expression tag	UNP P18669
D	260	HIS	-	expression tag	UNP P18669
D	261	HIS	-	expression tag	UNP P18669
D	262	HIS	-	expression tag	UNP P18669
E	255	LEU	-	expression tag	UNP P18669
E	256	GLU	-	expression tag	UNP P18669
E	257	HIS	-	expression tag	UNP P18669
E	258	HIS	-	expression tag	UNP P18669
E	259	HIS	-	expression tag	UNP P18669
E	260	HIS	-	expression tag	UNP P18669
E	261	HIS	-	expression tag	UNP P18669
E	262	HIS	-	expression tag	UNP P18669
F	255	LEU	-	expression tag	UNP P18669
F	256	GLU	-	expression tag	UNP P18669
F	257	HIS	-	expression tag	UNP P18669
F	258	HIS	-	expression tag	UNP P18669
F	259	HIS	-	expression tag	UNP P18669
F	260	HIS	-	expression tag	UNP P18669
F	261	HIS	-	expression tag	UNP P18669

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	262	HIS	-	expression tag	UNP P18669
G	255	LEU	-	expression tag	UNP P18669
G	256	GLU	-	expression tag	UNP P18669
G	257	HIS	-	expression tag	UNP P18669
G	258	HIS	-	expression tag	UNP P18669
G	259	HIS	-	expression tag	UNP P18669
G	260	HIS	-	expression tag	UNP P18669
G	261	HIS	-	expression tag	UNP P18669
G	262	HIS	-	expression tag	UNP P18669
H	255	LEU	-	expression tag	UNP P18669
H	256	GLU	-	expression tag	UNP P18669
H	257	HIS	-	expression tag	UNP P18669
H	258	HIS	-	expression tag	UNP P18669
H	259	HIS	-	expression tag	UNP P18669
H	260	HIS	-	expression tag	UNP P18669
H	261	HIS	-	expression tag	UNP P18669
H	262	HIS	-	expression tag	UNP P18669
I	255	LEU	-	expression tag	UNP P18669
I	256	GLU	-	expression tag	UNP P18669
I	257	HIS	-	expression tag	UNP P18669
I	258	HIS	-	expression tag	UNP P18669
I	259	HIS	-	expression tag	UNP P18669
I	260	HIS	-	expression tag	UNP P18669
I	261	HIS	-	expression tag	UNP P18669
I	262	HIS	-	expression tag	UNP P18669
J	255	LEU	-	expression tag	UNP P18669
J	256	GLU	-	expression tag	UNP P18669
J	257	HIS	-	expression tag	UNP P18669
J	258	HIS	-	expression tag	UNP P18669
J	259	HIS	-	expression tag	UNP P18669
J	260	HIS	-	expression tag	UNP P18669
J	261	HIS	-	expression tag	UNP P18669
J	262	HIS	-	expression tag	UNP P18669
K	255	LEU	-	expression tag	UNP P18669
K	256	GLU	-	expression tag	UNP P18669
K	257	HIS	-	expression tag	UNP P18669
K	258	HIS	-	expression tag	UNP P18669
K	259	HIS	-	expression tag	UNP P18669
K	260	HIS	-	expression tag	UNP P18669
K	261	HIS	-	expression tag	UNP P18669
K	262	HIS	-	expression tag	UNP P18669
L	255	LEU	-	expression tag	UNP P18669

Continued on next page...

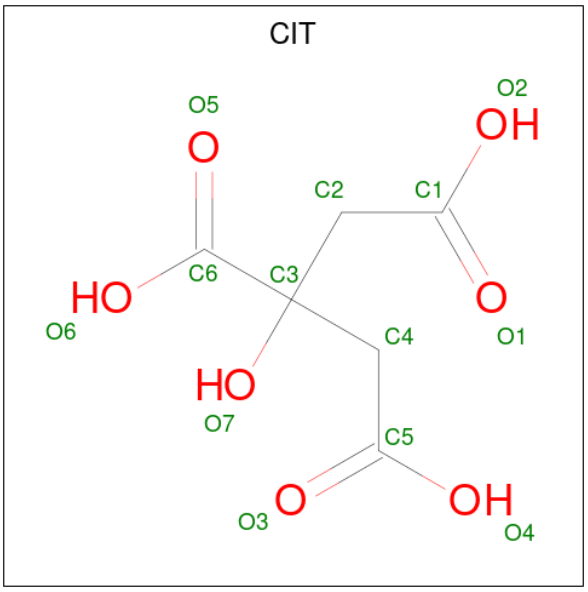
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	256	GLU	-	expression tag	UNP P18669
L	257	HIS	-	expression tag	UNP P18669
L	258	HIS	-	expression tag	UNP P18669
L	259	HIS	-	expression tag	UNP P18669
L	260	HIS	-	expression tag	UNP P18669
L	261	HIS	-	expression tag	UNP P18669
L	262	HIS	-	expression tag	UNP P18669

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	J	1	Total Cl 1 1	0	0
2	K	1	Total Cl 1 1	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0
3	D	1	Total C O 13 6 7	0	0
3	E	1	Total C O 13 6 7	0	0
3	F	1	Total C O 13 6 7	0	0
3	G	1	Total C O 13 6 7	0	0
3	H	1	Total C O 13 6 7	0	0
3	I	1	Total C O 13 6 7	0	0
3	J	1	Total C O 13 6 7	0	0
3	K	1	Total C O 13 6 7	0	0
3	L	1	Total C O 13 6 7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	43	Total O 43 43	0	0
4	B	45	Total O 45 45	0	0
4	C	21	Total O 21 21	0	0
4	D	33	Total O 33 33	0	0
4	E	17	Total O 17 17	0	0
4	F	27	Total O 27 27	0	0
4	G	12	Total O 12 12	0	0
4	H	18	Total O 18 18	0	0

Continued on next page...

Continued from previous page...

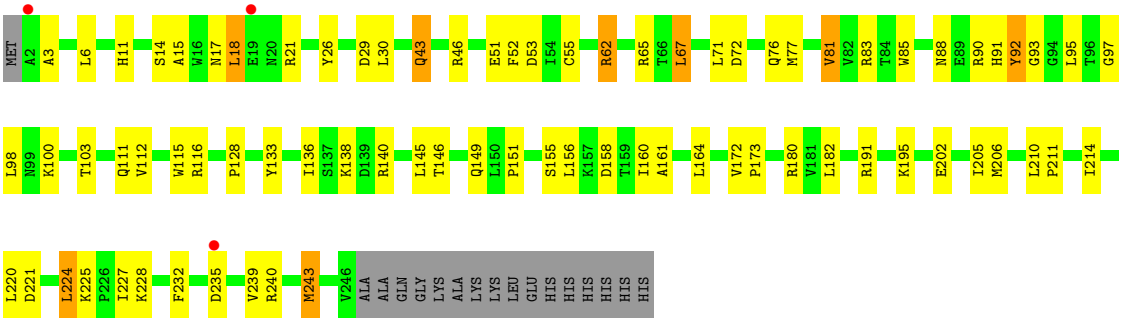
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	19	Total O 19 19	0	0
4	J	15	Total O 15 15	0	0
4	K	35	Total O 35 35	0	0
4	L	49	Total O 49 49	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

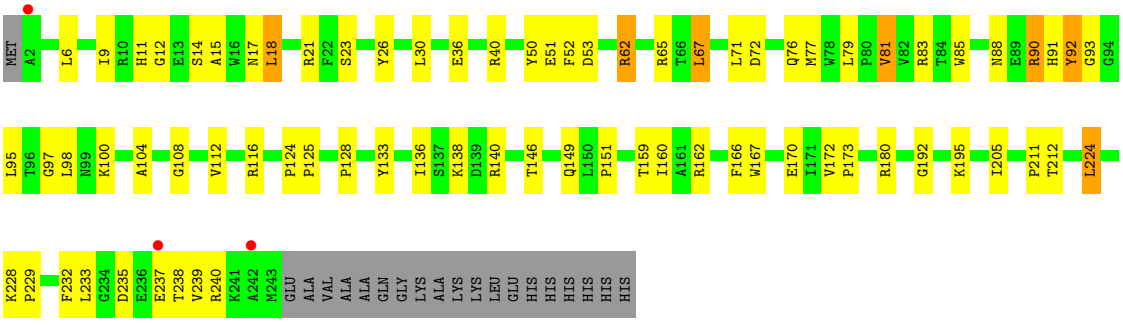
• Molecule 1: Phosphoglycerate mutase 1

Chain A:



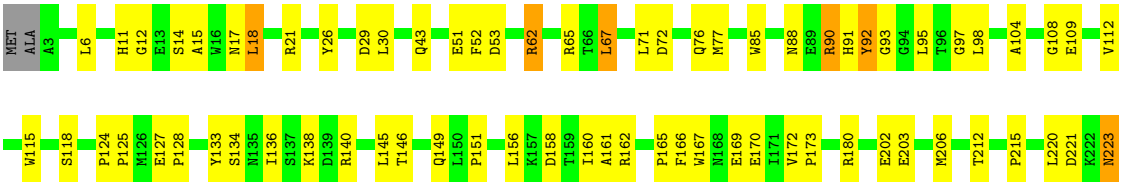
• Molecule 1: Phosphoglycerate mutase 1

Chain B:



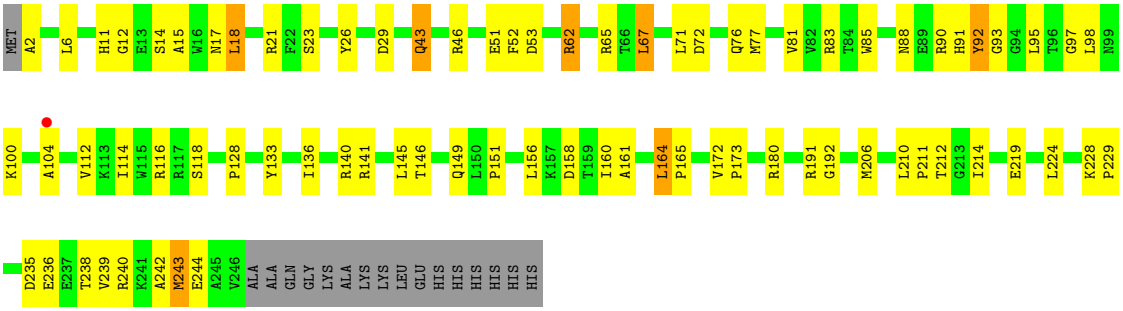
• Molecule 1: Phosphoglycerate mutase 1

Chain C:



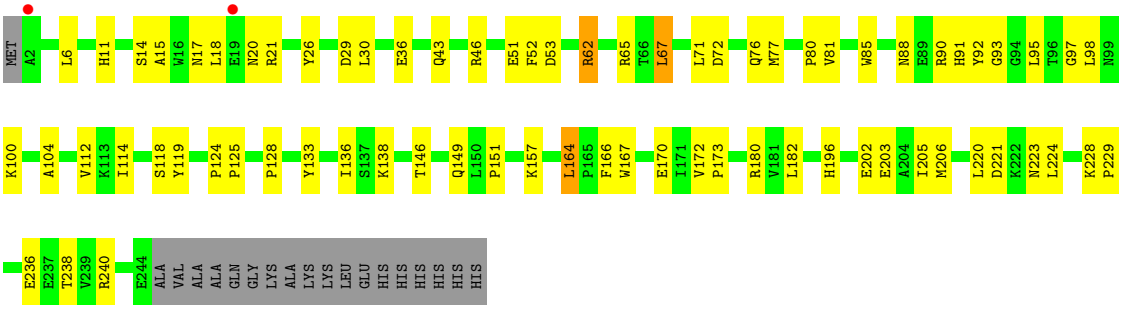
• Molecule 1: Phosphoglycerate mutase 1

Chain D:



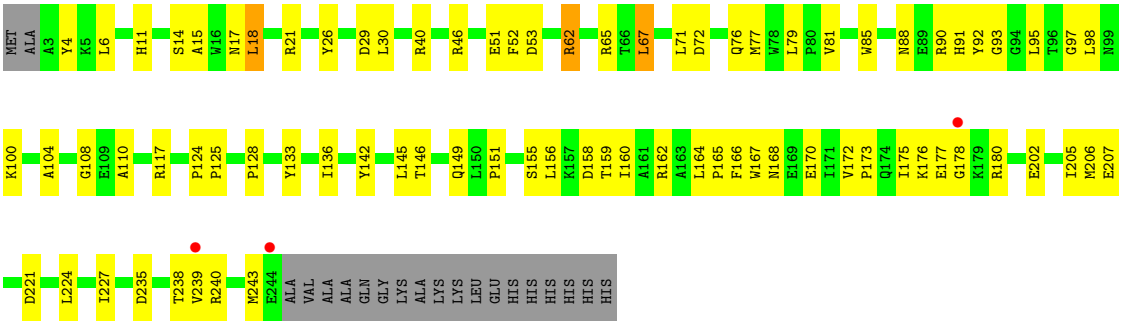
• Molecule 1: Phosphoglycerate mutase 1

Chain E:



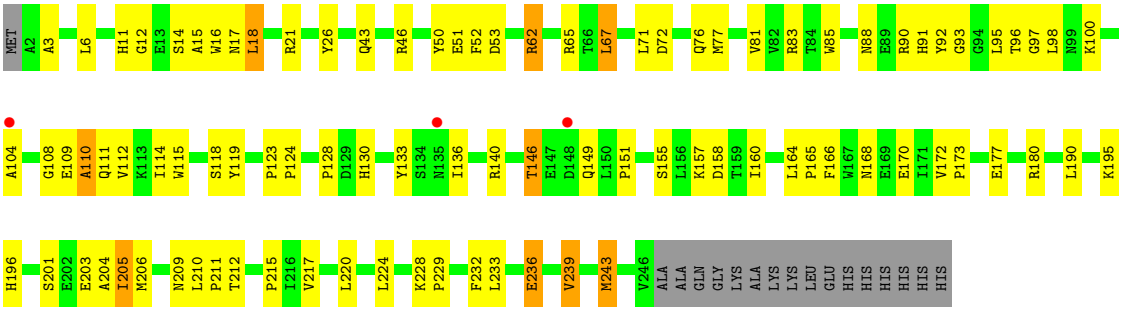
• Molecule 1: Phosphoglycerate mutase 1

Chain F:



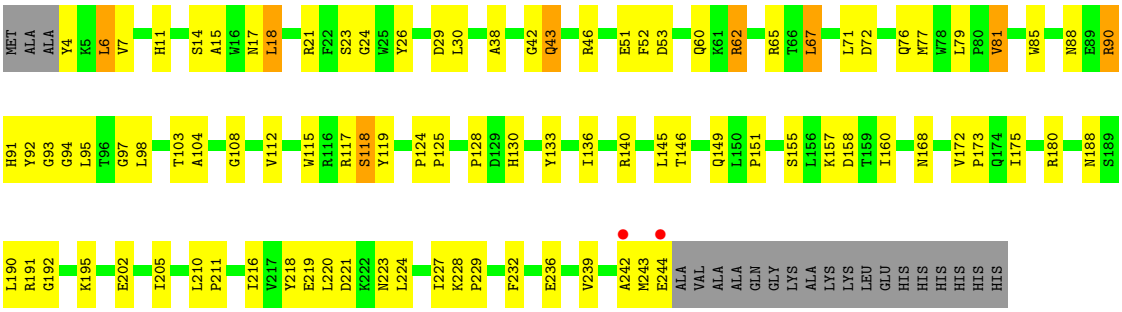
• Molecule 1: Phosphoglycerate mutase 1

Chain G:



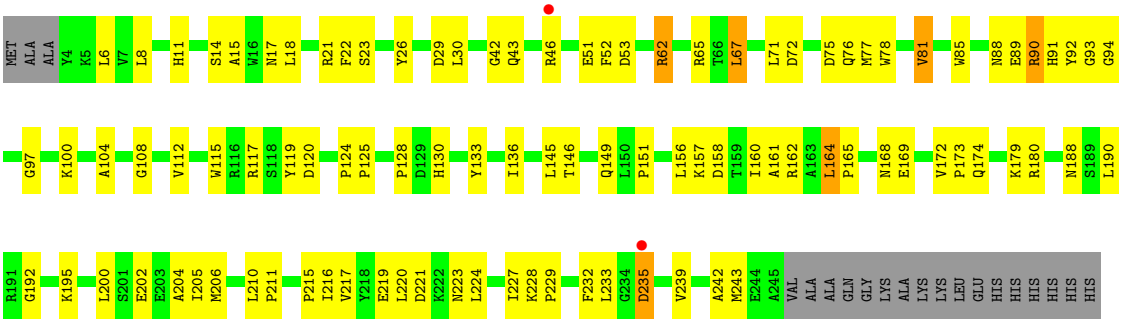
• Molecule 1: Phosphoglycerate mutase 1

Chain H:



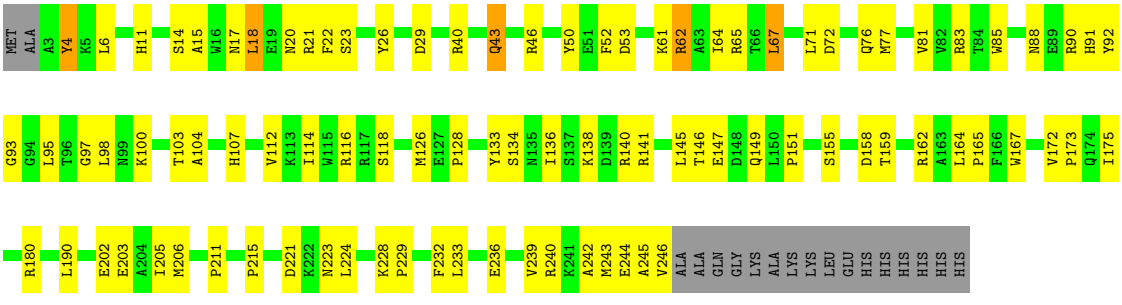
• Molecule 1: Phosphoglycerate mutase 1

Chain I:



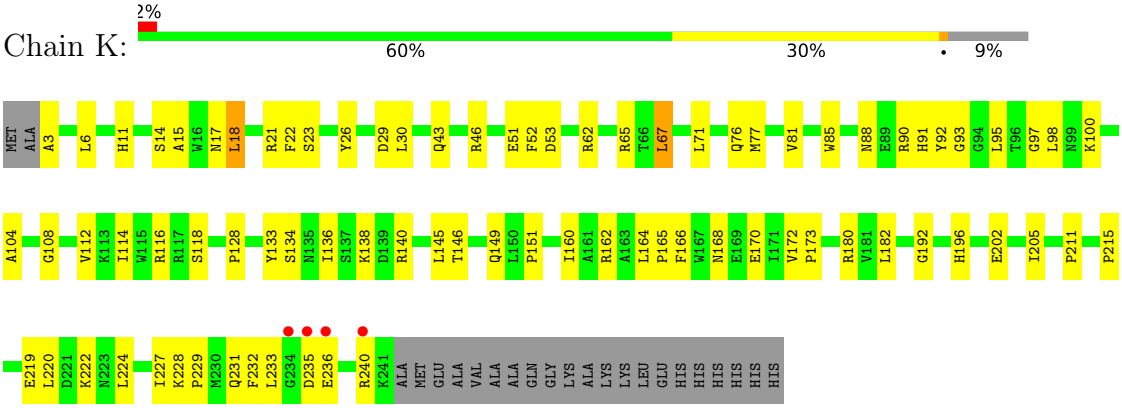
• Molecule 1: Phosphoglycerate mutase 1

Chain J:



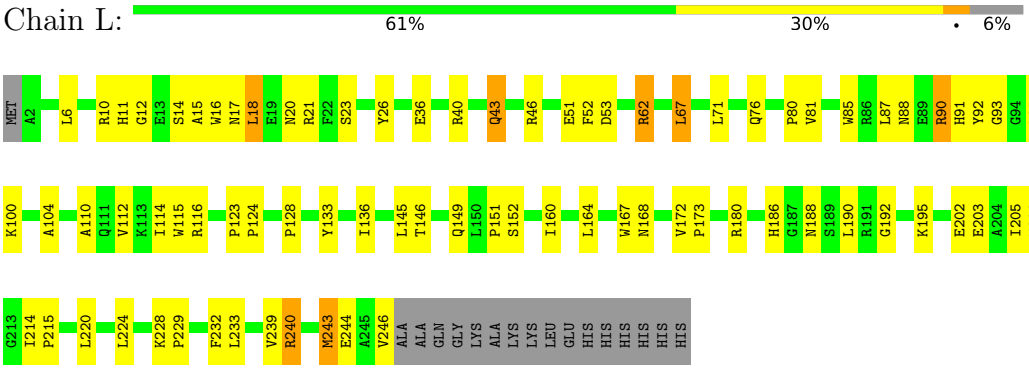
• Molecule 1: Phosphoglycerate mutase 1

Chain K:



• Molecule 1: Phosphoglycerate mutase 1

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	130.53Å 75.93Å 186.98Å 90.00° 94.42° 90.00°	Depositor
Resolution (Å)	29.91 – 2.80 29.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.91-2.80) 93.9 (29.91-2.80)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.272 0.224 , 0.261	Depositor DCC
R_{free} test set	8542 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	23286	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.38	0/1962	0.60	0/2671
1	B	0.38	0/1952	0.62	0/2655
1	C	0.36	0/1947	0.61	0/2652
1	D	0.37	0/1963	0.61	0/2673
1	E	0.37	0/1946	0.60	0/2650
1	F	0.36	0/1939	0.61	0/2641
1	G	0.36	0/1936	0.60	0/2641
1	H	0.37	0/1924	0.61	0/2621
1	I	0.37	0/1953	0.61	0/2657
1	J	0.37	0/1967	0.62	0/2676
1	K	0.37	0/1919	0.61	0/2612
1	L	0.38	0/1970	0.62	0/2679
All	All	0.37	0/23378	0.61	0/31828

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1913	0	1848	68	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1903	0	1845	64	0
1	C	1898	0	1827	63	0
1	D	1914	0	1843	66	0
1	E	1897	0	1822	62	0
1	F	1890	0	1819	77	0
1	G	1887	0	1786	83	0
1	H	1875	0	1800	84	0
1	I	1904	0	1844	96	0
1	J	1918	0	1858	83	0
1	K	1870	0	1806	72	0
1	L	1921	0	1865	73	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
3	A	13	0	5	1	0
3	B	13	0	5	2	0
3	C	13	0	5	1	0
3	D	13	0	5	2	0
3	E	13	0	5	0	0
3	F	13	0	5	1	0
3	G	13	0	5	1	0
3	H	13	0	5	2	0
3	I	13	0	5	1	0
3	J	13	0	5	2	0
3	K	13	0	5	3	0
3	L	13	0	5	3	0
4	A	43	0	0	2	0
4	B	45	0	0	1	0
4	C	21	0	0	1	0
4	D	33	0	0	3	0
4	E	17	0	0	3	0
4	F	27	0	0	5	0
4	G	12	0	0	1	0
4	H	18	0	0	2	0
4	I	19	0	0	2	0
4	J	15	0	0	1	0
4	K	35	0	0	8	0
4	L	49	0	0	3	0
All	All	23286	0	22023	861	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (861) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:HB2	1:A:205:ILE:HD12	1.22	1.11
1:H:195:LYS:HB2	1:H:205:ILE:HD12	1.34	1.09
1:A:91:HIS:HD2	1:A:93:GLY:H	1.12	0.98
1:F:206:MET:HE2	1:F:206:MET:HA	1.45	0.96
1:I:43:GLN:HE21	1:I:46:ARG:HH22	1.10	0.96
1:I:91:HIS:HD2	1:I:93:GLY:H	1.14	0.95
1:L:203:GLU:HA	1:L:206:MET:HE3	1.49	0.95
1:I:43:GLN:HE21	1:I:46:ARG:NH2	1.65	0.94
1:G:91:HIS:HD2	1:G:93:GLY:H	1.16	0.93
1:B:91:HIS:HD2	1:B:93:GLY:H	1.15	0.92
1:K:91:HIS:HD2	1:K:93:GLY:H	1.16	0.92
1:F:156:LEU:HD22	1:F:206:MET:HE1	1.52	0.92
1:H:91:HIS:HD2	1:H:93:GLY:H	1.17	0.91
1:G:26:TYR:HA	1:G:136:ILE:HD11	1.53	0.90
1:C:91:HIS:HD2	1:C:93:GLY:H	1.17	0.89
1:D:91:HIS:HD2	1:D:93:GLY:H	1.17	0.89
1:L:91:HIS:HD2	1:L:93:GLY:H	1.15	0.89
1:I:14:SER:H	1:I:17:ASN:HD22	1.21	0.89
1:A:14:SER:H	1:A:17:ASN:HD22	1.20	0.88
1:E:91:HIS:HD2	1:E:93:GLY:H	1.15	0.88
1:K:14:SER:H	1:K:17:ASN:HD22	1.22	0.88
1:G:14:SER:H	1:G:17:ASN:HD22	1.22	0.88
1:J:53:ASP:OD2	1:J:180:ARG:HD3	1.74	0.88
1:J:91:HIS:HD2	1:J:93:GLY:H	1.17	0.88
1:F:91:HIS:HD2	1:F:93:GLY:H	1.16	0.87
1:B:14:SER:H	1:B:17:ASN:HD22	1.22	0.87
1:H:14:SER:H	1:H:17:ASN:HD22	1.24	0.86
1:J:14:SER:H	1:J:17:ASN:HD22	1.22	0.85
1:E:14:SER:H	1:E:17:ASN:HD22	1.22	0.85
1:L:14:SER:H	1:L:17:ASN:HD22	1.25	0.85
1:F:156:LEU:HD22	1:F:206:MET:CE	2.07	0.85
1:I:146:THR:OG1	1:I:149:GLN:HG3	1.77	0.85
1:D:14:SER:H	1:D:17:ASN:HD22	1.22	0.84
1:C:14:SER:H	1:C:17:ASN:HD22	1.24	0.84
1:C:127:GLU:HG3	4:C:611:HOH:O	1.77	0.83
1:J:239:VAL:O	1:J:243:MET:HG2	1.78	0.82
1:F:14:SER:H	1:F:17:ASN:HD22	1.24	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:52:PHE:H	1:I:76:GLN:HE22	1.29	0.80
1:E:52:PHE:H	1:E:76:GLN:HE22	1.30	0.80
1:G:52:PHE:H	1:G:76:GLN:HE22	1.30	0.79
1:I:43:GLN:NE2	1:I:46:ARG:HH22	1.79	0.79
1:L:52:PHE:H	1:L:76:GLN:HE22	1.30	0.79
1:J:52:PHE:H	1:J:76:GLN:HE22	1.30	0.79
1:H:52:PHE:H	1:H:76:GLN:HE22	1.30	0.78
1:A:52:PHE:H	1:A:76:GLN:HE22	1.31	0.78
1:E:36:GLU:HG3	4:E:621:HOH:O	1.81	0.78
1:C:52:PHE:H	1:C:76:GLN:HE22	1.32	0.78
1:D:52:PHE:H	1:D:76:GLN:HE22	1.32	0.77
1:L:160:ILE:HG23	1:L:164:LEU:HD23	1.65	0.77
1:D:240:ARG:HA	1:D:243:MET:HB2	1.65	0.77
1:G:43:GLN:HE21	1:G:46:ARG:NH1	1.82	0.77
1:F:52:PHE:H	1:F:76:GLN:HE22	1.32	0.76
1:K:52:PHE:H	1:K:76:GLN:HE22	1.31	0.76
1:B:52:PHE:H	1:B:76:GLN:HE22	1.32	0.76
1:F:26:TYR:HA	1:F:136:ILE:HD11	1.68	0.76
1:F:172:VAL:HG13	1:F:224:LEU:HD11	1.69	0.75
1:I:232:PHE:HB2	1:I:239:VAL:HG23	1.66	0.75
1:I:217:VAL:HG21	1:I:233:LEU:HD21	1.68	0.75
1:L:123:PRO:HD3	4:L:658:HOH:O	1.85	0.74
1:I:172:VAL:HG13	1:I:224:LEU:HD11	1.69	0.74
1:J:4:TYR:CD1	1:J:175:ILE:HG22	2.22	0.74
1:E:26:TYR:HA	1:E:136:ILE:HD11	1.70	0.74
1:F:206:MET:HA	1:F:206:MET:CE	2.17	0.74
1:L:104:ALA:HA	1:L:112:VAL:HG21	1.70	0.74
1:D:53:ASP:OD2	1:D:180:ARG:HD3	1.87	0.73
1:L:21:ARG:HD2	1:L:97:GLY:O	1.88	0.73
1:J:172:VAL:HG13	1:J:224:LEU:HD11	1.69	0.73
1:D:235:ASP:O	1:D:239:VAL:HG12	1.87	0.73
1:G:26:TYR:HA	1:G:136:ILE:CD1	2.18	0.73
1:K:227:ILE:HD12	1:K:228:LYS:HG2	1.71	0.73
1:G:177:GLU:HG2	1:J:40:ARG:HH22	1.53	0.73
1:B:146:THR:OG1	1:B:149:GLN:HG3	1.89	0.72
1:J:43:GLN:HG3	1:J:46:ARG:NH2	2.04	0.72
1:L:243:MET:HE3	1:L:243:MET:HA	1.70	0.72
1:I:165:PRO:O	1:I:169:GLU:HG3	1.90	0.72
1:A:91:HIS:CD2	1:A:93:GLY:H	2.03	0.71
1:K:53:ASP:OD2	1:K:180:ARG:HD3	1.89	0.71
1:H:172:VAL:HG13	1:H:224:LEU:HD11	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:ARG:HD2	1:H:97:GLY:O	1.90	0.71
1:E:53:ASP:OD2	1:E:180:ARG:HD3	1.90	0.71
1:G:164:LEU:HD11	1:G:196:HIS:HB2	1.72	0.71
1:I:62:ARG:NH1	4:I:620:HOH:O	2.23	0.71
1:I:221:ASP:OD1	1:I:223:ASN:N	2.24	0.71
1:C:85:TRP:CE2	1:C:145:LEU:HD21	2.26	0.70
1:F:117:ARG:HH21	1:F:207:GLU:HG2	1.56	0.70
1:G:115:TRP:CD1	1:G:123:PRO:HA	2.26	0.70
1:D:172:VAL:HG13	1:D:224:LEU:HD11	1.73	0.70
1:J:4:TYR:HD1	1:J:175:ILE:HG22	1.54	0.70
1:G:146:THR:OG1	1:G:149:GLN:HG3	1.91	0.70
1:J:4:TYR:HD1	1:J:175:ILE:CG2	2.04	0.69
1:L:146:THR:OG1	1:L:149:GLN:HG3	1.91	0.69
1:B:235:ASP:O	1:B:239:VAL:HG12	1.91	0.69
1:A:146:THR:OG1	1:A:149:GLN:HG3	1.92	0.69
1:H:51:GLU:HB2	1:H:180:ARG:NH2	2.08	0.69
1:H:104:ALA:O	1:H:108:GLY:N	2.24	0.69
1:C:26:TYR:HA	1:C:136:ILE:HD11	1.74	0.69
1:E:146:THR:OG1	1:E:149:GLN:HG3	1.93	0.69
1:I:53:ASP:OD2	1:I:180:ARG:HD3	1.93	0.69
1:B:21:ARG:HD2	1:B:97:GLY:O	1.93	0.68
1:D:156:LEU:HD23	1:D:206:MET:SD	2.34	0.68
1:G:43:GLN:HG3	1:G:46:ARG:NH2	2.07	0.68
1:G:172:VAL:HG13	1:G:224:LEU:HD11	1.75	0.68
1:I:164:LEU:HD12	1:I:168:ASN:HD21	1.58	0.68
1:I:239:VAL:O	1:I:243:MET:HG2	1.94	0.68
1:A:227:ILE:HG13	1:A:228:LYS:HG2	1.75	0.67
1:B:112:VAL:O	1:B:116:ARG:HG3	1.95	0.67
1:I:52:PHE:H	1:I:76:GLN:NE2	1.92	0.67
1:J:146:THR:OG1	1:J:149:GLN:HG3	1.95	0.67
1:E:43:GLN:CD	1:E:46:ARG:NH2	2.48	0.67
1:E:52:PHE:H	1:E:76:GLN:NE2	1.92	0.67
1:G:53:ASP:OD2	1:G:180:ARG:HD3	1.95	0.67
1:G:115:TRP:CE2	1:G:124:PRO:HD3	2.29	0.67
1:I:202:GLU:O	1:I:205:ILE:HG22	1.95	0.67
1:B:91:HIS:CD2	1:B:93:GLY:H	2.07	0.66
1:L:12:GLY:HA2	1:L:212:THR:HB	1.78	0.66
1:I:243:MET:HE3	1:I:243:MET:HA	1.78	0.66
1:F:21:ARG:HD2	1:F:97:GLY:O	1.96	0.66
1:L:52:PHE:H	1:L:76:GLN:NE2	1.93	0.66
1:E:203:GLU:HA	1:E:206:MET:CE	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:52:PHE:H	1:J:76:GLN:NE2	1.93	0.66
1:F:67:LEU:HD22	1:F:71:LEU:HG	1.78	0.66
1:G:43:GLN:HE21	1:G:46:ARG:CZ	2.07	0.66
1:J:91:HIS:CD2	1:J:93:GLY:H	2.07	0.66
1:L:116:ARG:HD2	3:L:612:CIT:O1	1.95	0.66
1:L:91:HIS:CD2	1:L:93:GLY:H	2.07	0.65
1:A:52:PHE:H	1:A:76:GLN:NE2	1.92	0.65
1:F:52:PHE:H	1:F:76:GLN:NE2	1.94	0.65
1:F:160:ILE:O	1:F:164:LEU:HD23	1.96	0.65
1:J:147:GLU:OE1	1:J:147:GLU:HA	1.93	0.65
1:D:67:LEU:HD22	1:D:71:LEU:HG	1.79	0.65
1:D:91:HIS:CD2	1:D:93:GLY:H	2.08	0.65
1:G:52:PHE:H	1:G:76:GLN:NE2	1.94	0.65
1:F:91:HIS:CD2	1:F:93:GLY:H	2.07	0.65
1:A:14:SER:N	1:A:17:ASN:HD22	1.94	0.65
1:A:26:TYR:HA	1:A:136:ILE:HD11	1.79	0.65
1:I:91:HIS:CD2	1:I:93:GLY:H	2.06	0.65
1:A:191:ARG:HB3	1:A:205:ILE:HD11	1.79	0.65
1:B:52:PHE:H	1:B:76:GLN:NE2	1.95	0.65
1:C:52:PHE:H	1:C:76:GLN:NE2	1.95	0.65
1:L:26:TYR:HA	1:L:136:ILE:HD11	1.78	0.65
1:B:100:LYS:HD3	1:B:116:ARG:NH1	2.12	0.64
1:G:243:MET:HE2	1:G:243:MET:HA	1.79	0.64
1:H:52:PHE:H	1:H:76:GLN:NE2	1.94	0.64
1:K:52:PHE:H	1:K:76:GLN:NE2	1.95	0.64
1:H:91:HIS:CD2	1:H:93:GLY:H	2.08	0.64
1:E:21:ARG:HD2	1:E:97:GLY:O	1.98	0.64
1:D:43:GLN:HG3	1:D:46:ARG:NH2	2.13	0.64
1:E:67:LEU:HD22	1:E:71:LEU:HG	1.79	0.64
1:C:21:ARG:HD2	1:C:97:GLY:O	1.97	0.64
1:F:168:ASN:O	1:F:173:PRO:HD3	1.98	0.64
1:J:126:MET:HA	4:J:614:HOH:O	1.97	0.64
1:L:51:GLU:HB2	1:L:180:ARG:NH2	2.12	0.64
1:D:14:SER:N	1:D:17:ASN:HD22	1.95	0.64
1:D:146:THR:OG1	1:D:149:GLN:HG3	1.97	0.64
1:G:67:LEU:HD22	1:G:71:LEU:HG	1.79	0.64
1:H:67:LEU:HD22	1:H:71:LEU:HG	1.80	0.64
1:D:52:PHE:H	1:D:76:GLN:NE2	1.95	0.64
1:F:53:ASP:OD2	1:F:180:ARG:HD3	1.96	0.64
1:G:215:PRO:HB2	1:G:233:LEU:HB2	1.79	0.64
1:B:53:ASP:OD2	1:B:180:ARG:HD3	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:TRP:NE1	1:A:145:LEU:HD21	2.12	0.63
1:B:239:VAL:HG13	1:B:240:ARG:H	1.63	0.63
1:H:216:ILE:HG12	1:H:232:PHE:HE2	1.64	0.63
1:J:26:TYR:HA	1:J:136:ILE:HD11	1.79	0.63
1:L:67:LEU:HD22	1:L:71:LEU:HG	1.81	0.63
1:J:14:SER:N	1:J:17:ASN:HD22	1.96	0.63
1:J:67:LEU:HD22	1:J:71:LEU:HG	1.80	0.63
1:K:211:PRO:HG2	1:K:232:PHE:CE1	2.33	0.63
1:E:203:GLU:HA	1:E:206:MET:HE2	1.81	0.63
1:A:67:LEU:HD22	1:A:71:LEU:HG	1.81	0.62
1:A:235:ASP:O	1:A:239:VAL:HG12	1.98	0.62
1:J:22:PHE:CE1	1:J:116:ARG:HD3	2.34	0.62
1:E:91:HIS:CD2	1:E:93:GLY:H	2.07	0.62
1:I:14:SER:N	1:I:17:ASN:HD22	1.95	0.62
1:B:14:SER:N	1:B:17:ASN:HD22	1.95	0.62
1:I:26:TYR:HA	1:I:136:ILE:HD11	1.81	0.62
1:J:211:PRO:HG2	1:J:232:PHE:CE1	2.35	0.62
1:H:26:TYR:HA	1:H:136:ILE:HD11	1.82	0.62
1:I:158:ASP:O	1:I:161:ALA:HB3	2.00	0.62
1:I:243:MET:HA	1:I:243:MET:CE	2.30	0.62
1:K:67:LEU:HD22	1:K:71:LEU:HG	1.82	0.62
1:K:100:LYS:NZ	3:K:611:CIT:H21	2.14	0.62
1:I:67:LEU:HD22	1:I:71:LEU:HG	1.80	0.62
1:D:114:ILE:O	1:D:118:SER:HB3	2.00	0.62
1:K:91:HIS:CD2	1:K:93:GLY:H	2.07	0.62
1:L:36:GLU:HG3	4:L:615:HOH:O	2.00	0.62
1:C:91:HIS:CD2	1:C:93:GLY:H	2.09	0.62
1:E:14:SER:N	1:E:17:ASN:HD22	1.96	0.62
1:B:67:LEU:HD22	1:B:71:LEU:HG	1.82	0.61
1:K:26:TYR:HA	1:K:136:ILE:HD11	1.82	0.61
1:K:146:THR:OG1	1:K:149:GLN:HG3	2.00	0.61
1:I:227:ILE:HD11	1:I:228:LYS:HE3	1.82	0.61
1:L:228:LYS:HB2	1:L:229:PRO:HD2	1.81	0.61
1:E:26:TYR:HA	1:E:136:ILE:CD1	2.31	0.61
1:A:51:GLU:HB2	1:A:180:ARG:NH2	2.16	0.61
1:F:146:THR:OG1	1:F:149:GLN:HG3	2.00	0.61
1:I:235:ASP:O	1:I:239:VAL:HG12	2.00	0.61
1:K:11:HIS:NE2	1:K:62:ARG:HD2	2.14	0.61
1:G:119:TYR:HB2	1:G:206:MET:SD	2.41	0.61
1:H:14:SER:N	1:H:17:ASN:HD22	1.97	0.61
1:B:166:PHE:CE1	1:B:170:GLU:HG3	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:15:ALA:O	1:J:18:LEU:HD23	2.00	0.61
1:I:75:ASP:OD2	1:J:61:LYS:HE3	2.01	0.60
1:C:15:ALA:O	1:C:18:LEU:HD23	2.02	0.60
1:F:91:HIS:HD2	1:F:93:GLY:N	1.95	0.60
1:B:100:LYS:HD3	1:B:116:ARG:HH12	1.66	0.60
1:C:53:ASP:OD2	1:C:180:ARG:HD3	2.00	0.60
1:F:11:HIS:NE2	1:F:62:ARG:HD2	2.16	0.60
1:L:203:GLU:CA	1:L:206:MET:HE3	2.29	0.60
1:A:53:ASP:OD2	1:A:180:ARG:HD3	2.01	0.60
1:G:51:GLU:HB2	1:G:180:ARG:NH2	2.16	0.60
1:L:14:SER:N	1:L:17:ASN:HD22	1.97	0.60
1:B:51:GLU:HB2	1:B:180:ARG:NH2	2.16	0.60
1:H:15:ALA:O	1:H:18:LEU:HD23	2.02	0.60
1:I:91:HIS:HD2	1:I:93:GLY:N	1.94	0.60
1:F:162:ARG:C	1:F:165:PRO:HD2	2.23	0.60
1:I:21:ARG:HD2	1:I:97:GLY:O	2.02	0.60
1:L:36:GLU:O	1:L:40:ARG:HG3	2.02	0.60
1:A:85:TRP:CE2	1:A:145:LEU:HD21	2.37	0.59
1:G:15:ALA:O	1:G:18:LEU:HD23	2.02	0.59
1:D:26:TYR:HA	1:D:136:ILE:HD11	1.83	0.59
1:C:67:LEU:HD22	1:C:71:LEU:HG	1.84	0.59
1:H:242:ALA:C	1:H:244:GLU:H	2.06	0.59
1:E:236:GLU:C	1:E:238:THR:H	2.05	0.59
1:C:167:TRP:O	1:C:172:VAL:HG23	2.03	0.59
1:G:149:GLN:O	1:G:151:PRO:HD3	2.03	0.59
1:J:104:ALA:HA	1:J:112:VAL:HG21	1.85	0.59
1:A:91:HIS:HD2	1:A:93:GLY:N	1.93	0.59
1:C:14:SER:N	1:C:17:ASN:HD22	1.96	0.59
1:F:227:ILE:HG22	1:F:227:ILE:O	2.03	0.59
1:I:52:PHE:O	1:J:140:ARG:NH1	2.36	0.59
1:K:215:PRO:HB2	1:K:233:LEU:HB2	1.85	0.59
1:G:104:ALA:HB1	1:G:109:GLU:OE1	2.03	0.58
1:I:168:ASN:O	1:I:173:PRO:HD3	2.03	0.58
1:K:14:SER:N	1:K:17:ASN:HD22	1.95	0.58
1:L:202:GLU:O	1:L:205:ILE:HG22	2.03	0.58
1:E:167:TRP:O	1:E:172:VAL:HG23	2.03	0.58
1:G:14:SER:N	1:G:17:ASN:HD22	1.95	0.58
1:H:146:THR:OG1	1:H:149:GLN:HG3	2.02	0.58
1:I:75:ASP:OD2	1:J:61:LYS:CE	2.51	0.58
1:B:26:TYR:HA	1:B:136:ILE:HD11	1.85	0.58
1:G:12:GLY:HA2	1:G:212:THR:HB	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:HIS:HD2	1:G:93:GLY:N	1.95	0.58
1:L:15:ALA:O	1:L:18:LEU:HD23	2.03	0.58
1:I:11:HIS:NE2	1:I:62:ARG:HD2	2.18	0.58
1:C:146:THR:OG1	1:C:149:GLN:HG3	2.03	0.58
1:H:160:ILE:HG12	1:H:192:GLY:HA2	1.85	0.58
1:J:21:ARG:HD2	1:J:97:GLY:O	2.03	0.58
1:F:14:SER:N	1:F:17:ASN:HD22	1.96	0.58
1:G:21:ARG:HD2	1:G:97:GLY:O	2.04	0.58
1:E:202:GLU:O	1:E:206:MET:HG3	2.04	0.57
1:I:15:ALA:O	1:I:18:LEU:HD23	2.04	0.57
1:J:149:GLN:O	1:J:151:PRO:HD3	2.04	0.57
1:B:15:ALA:O	1:B:18:LEU:HD23	2.04	0.57
1:H:216:ILE:HG12	1:H:232:PHE:CE2	2.38	0.57
1:H:236:GLU:HA	1:H:239:VAL:CG1	2.34	0.57
1:D:15:ALA:O	1:D:18:LEU:HD23	2.04	0.57
1:A:202:GLU:O	1:A:206:MET:HG3	2.04	0.57
1:G:91:HIS:CD2	1:G:93:GLY:H	2.07	0.57
1:L:172:VAL:HG13	1:L:224:LEU:HD11	1.86	0.57
1:F:11:HIS:CE1	1:F:62:ARG:HD2	2.39	0.57
1:G:85:TRP:O	1:G:88:ASN:HB2	2.04	0.57
1:H:172:VAL:HG13	1:H:224:LEU:CD1	2.35	0.57
1:A:112:VAL:HG13	1:A:116:ARG:HG3	1.86	0.57
1:C:134:SER:O	1:C:138:LYS:HB2	2.05	0.57
1:H:11:HIS:NE2	1:H:62:ARG:HD2	2.20	0.57
1:D:242:ALA:C	1:D:244:GLU:H	2.08	0.56
1:G:43:GLN:NE2	1:G:46:ARG:HH12	2.03	0.56
1:G:65:ARG:NH2	1:H:72:ASP:OD1	2.37	0.56
1:I:149:GLN:O	1:I:151:PRO:HD3	2.04	0.56
1:L:149:GLN:O	1:L:151:PRO:HD3	2.05	0.56
1:C:52:PHE:O	1:D:140:ARG:NH1	2.36	0.56
1:H:85:TRP:NE1	1:H:145:LEU:HD21	2.20	0.56
1:F:15:ALA:O	1:F:18:LEU:HD23	2.05	0.56
1:F:155:SER:H	1:F:158:ASP:HB2	1.71	0.56
1:K:140:ARG:HD3	4:K:635:HOH:O	2.03	0.56
1:F:205:ILE:HG23	1:F:206:MET:HE3	1.87	0.56
1:H:91:HIS:HD2	1:H:93:GLY:N	1.97	0.56
1:G:211:PRO:HG2	1:G:232:PHE:CE1	2.41	0.56
1:J:85:TRP:O	1:J:88:ASN:HB2	2.05	0.56
1:L:160:ILE:HG23	1:L:164:LEU:CD2	2.34	0.56
1:F:166:PHE:CE1	1:F:170:GLU:HG3	2.41	0.56
1:J:155:SER:H	1:J:158:ASP:HB2	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:202:GLU:O	1:L:206:MET:HG3	2.06	0.56
1:G:43:GLN:NE2	1:G:46:ARG:NH1	2.53	0.56
1:E:11:HIS:NE2	1:E:62:ARG:HD2	2.21	0.56
1:L:85:TRP:CE2	1:L:145:LEU:HD21	2.41	0.56
1:A:149:GLN:O	1:A:151:PRO:HD3	2.06	0.55
1:C:172:VAL:HG13	1:C:224:LEU:HD11	1.88	0.55
1:D:91:HIS:HD2	1:D:93:GLY:N	1.96	0.55
1:H:43:GLN:HG3	1:H:46:ARG:NH2	2.21	0.55
1:L:90:ARG:NH2	4:L:658:HOH:O	2.39	0.55
1:A:21:ARG:HD2	1:A:97:GLY:O	2.06	0.55
1:D:239:VAL:HG22	1:D:239:VAL:O	2.07	0.55
1:E:149:GLN:O	1:E:151:PRO:HD3	2.06	0.55
1:F:30:LEU:HD12	1:F:65:ARG:HG2	1.88	0.55
1:C:11:HIS:NE2	1:C:62:ARG:HD2	2.22	0.55
1:C:26:TYR:HA	1:C:136:ILE:CD1	2.36	0.55
1:F:40:ARG:NH2	4:F:612:HOH:O	2.39	0.55
1:G:236:GLU:HA	1:G:239:VAL:HG13	1.87	0.55
1:I:85:TRP:O	1:I:88:ASN:HB2	2.07	0.55
1:J:114:ILE:O	1:J:118:SER:HB3	2.07	0.55
1:F:221:ASP:HB3	1:F:227:ILE:HD11	1.89	0.55
1:I:72:ASP:CG	1:J:65:ARG:NH2	2.60	0.55
1:K:21:ARG:HD2	1:K:97:GLY:O	2.05	0.55
1:K:166:PHE:CE1	1:K:170:GLU:HG3	2.41	0.55
1:F:85:TRP:O	1:F:88:ASN:HB2	2.07	0.55
1:H:85:TRP:O	1:H:88:ASN:HB2	2.07	0.55
1:E:11:HIS:CE1	1:E:62:ARG:HD2	2.42	0.55
1:F:26:TYR:HA	1:F:136:ILE:CD1	2.36	0.55
1:F:202:GLU:HG3	4:F:619:HOH:O	2.07	0.55
1:B:11:HIS:NE2	1:B:62:ARG:HD2	2.22	0.54
1:A:85:TRP:O	1:A:88:ASN:HB2	2.07	0.54
1:D:62:ARG:NH1	4:D:606:HOH:O	2.39	0.54
1:L:115:TRP:CE2	1:L:124:PRO:HD3	2.42	0.54
1:D:156:LEU:HD22	1:D:191:ARG:HH11	1.73	0.54
1:K:15:ALA:O	1:K:18:LEU:HD23	2.07	0.54
1:K:85:TRP:O	1:K:88:ASN:HB2	2.07	0.54
1:D:156:LEU:CD2	1:D:206:MET:SD	2.96	0.54
1:J:159:THR:HG23	1:J:162:ARG:NH2	2.22	0.54
1:C:51:GLU:HB2	1:C:180:ARG:NH2	2.21	0.54
1:D:85:TRP:O	1:D:88:ASN:HB2	2.07	0.54
1:D:149:GLN:O	1:D:151:PRO:HD3	2.08	0.54
1:F:62:ARG:NH2	4:F:629:HOH:O	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:168:ASN:O	1:H:173:PRO:HD3	2.08	0.54
1:H:236:GLU:HA	1:H:239:VAL:HG12	1.88	0.54
1:J:116:ARG:HD2	3:J:610:CIT:O1	2.08	0.54
1:K:219:GLU:O	1:K:227:ILE:HG13	2.08	0.54
1:F:117:ARG:NH2	1:F:207:GLU:HG2	2.22	0.54
1:H:11:HIS:CE1	1:H:62:ARG:HD2	2.43	0.54
1:F:104:ALA:O	1:F:108:GLY:N	2.41	0.54
1:F:146:THR:HG23	1:F:149:GLN:OE1	2.08	0.54
1:D:100:LYS:HD3	1:D:116:ARG:NH1	2.22	0.54
1:I:77:MET:HE1	1:J:65:ARG:HH22	1.71	0.54
4:K:616:HOH:O	1:L:80:PRO:HA	2.08	0.54
1:A:11:HIS:NE2	1:A:62:ARG:HD2	2.22	0.53
1:G:203:GLU:HA	1:G:206:MET:HE3	1.90	0.53
1:J:203:GLU:HA	1:J:206:MET:CE	2.39	0.53
1:B:91:HIS:HD2	1:B:93:GLY:N	1.95	0.53
1:J:236:GLU:O	1:J:239:VAL:HG12	2.08	0.53
1:L:11:HIS:NE2	1:L:62:ARG:HD2	2.24	0.53
1:C:85:TRP:NE1	1:C:145:LEU:HD21	2.23	0.53
1:C:85:TRP:O	1:C:88:ASN:HB2	2.08	0.53
1:C:236:GLU:O	1:C:239:VAL:HG12	2.08	0.53
1:D:228:LYS:HB2	1:D:229:PRO:HD2	1.89	0.53
1:K:227:ILE:HD12	1:K:227:ILE:C	2.28	0.53
1:C:91:HIS:HD2	1:C:93:GLY:N	1.97	0.53
1:C:104:ALA:HA	1:C:112:VAL:HG21	1.90	0.53
1:I:104:ALA:O	1:I:108:GLY:N	2.35	0.53
1:B:92:TYR:CE2	3:B:602:CIT:H22	2.43	0.53
1:E:30:LEU:HD12	1:E:65:ARG:HG2	1.91	0.53
1:E:85:TRP:O	1:E:88:ASN:HB2	2.08	0.53
1:L:90:ARG:HB3	1:L:188:ASN:HD22	1.74	0.53
1:C:221:ASP:OD1	1:C:223:ASN:N	2.41	0.53
1:H:149:GLN:O	1:H:151:PRO:HD3	2.08	0.53
1:I:228:LYS:HB2	1:I:229:PRO:HD2	1.90	0.53
1:J:134:SER:HA	1:J:138:LYS:HB2	1.90	0.53
1:I:94:GLY:HA2	1:I:130:HIS:CD2	2.44	0.52
1:J:221:ASP:OD1	1:J:223:ASN:N	2.37	0.52
1:K:30:LEU:HD12	1:K:65:ARG:HG2	1.90	0.52
1:B:159:THR:O	1:B:162:ARG:HD2	2.10	0.52
1:G:220:LEU:HB3	1:G:224:LEU:HA	1.91	0.52
1:L:43:GLN:HG3	1:L:46:ARG:NH2	2.24	0.52
1:F:85:TRP:NE1	1:F:145:LEU:HD21	2.24	0.52
1:G:72:ASP:OD1	1:H:65:ARG:NH2	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:72:ASP:OD2	1:I:77:MET:HE1	2.10	0.52
1:I:119:TYR:CD1	1:I:156:LEU:HD23	2.45	0.52
1:A:15:ALA:O	1:A:18:LEU:HD23	2.10	0.52
1:A:30:LEU:HD12	1:A:65:ARG:HG2	1.91	0.52
1:B:239:VAL:HG13	1:B:240:ARG:N	2.24	0.52
1:E:51:GLU:HB2	1:E:180:ARG:NH2	2.24	0.52
1:F:149:GLN:O	1:F:151:PRO:HD3	2.10	0.52
1:H:155:SER:H	1:H:158:ASP:HB2	1.74	0.52
1:C:149:GLN:O	1:C:151:PRO:HD3	2.10	0.52
1:F:51:GLU:HB2	1:F:180:ARG:NH2	2.24	0.52
1:K:85:TRP:NE1	1:K:145:LEU:HD21	2.25	0.52
1:E:43:GLN:OE1	1:E:46:ARG:NH2	2.43	0.52
1:K:134:SER:O	1:K:138:LYS:HB2	2.10	0.52
1:B:149:GLN:O	1:B:151:PRO:HD3	2.10	0.51
1:H:51:GLU:HB2	1:H:180:ARG:HH21	1.74	0.51
1:L:168:ASN:O	1:L:173:PRO:HD3	2.09	0.51
1:B:11:HIS:CE1	1:B:62:ARG:HD2	2.45	0.51
1:K:77:MET:HG3	4:K:644:HOH:O	2.11	0.51
1:B:104:ALA:O	1:B:108:GLY:N	2.40	0.51
1:D:85:TRP:CD1	1:D:145:LEU:HD21	2.46	0.51
1:F:117:ARG:O	1:F:117:ARG:HG2	2.10	0.51
1:D:21:ARG:HD2	1:D:97:GLY:O	2.09	0.51
1:F:62:ARG:NE	4:F:629:HOH:O	2.36	0.51
1:I:30:LEU:HD12	1:I:65:ARG:HG2	1.90	0.51
1:I:117:ARG:O	1:I:206:MET:HG2	2.11	0.51
1:K:104:ALA:HA	1:K:112:VAL:HG21	1.91	0.51
1:I:11:HIS:CE1	1:I:62:ARG:HD2	2.46	0.51
1:I:221:ASP:OD1	1:I:223:ASN:HB2	2.11	0.51
1:L:85:TRP:NE1	1:L:145:LEU:HD21	2.24	0.51
1:D:11:HIS:NE2	1:D:62:ARG:HD2	2.26	0.51
1:F:235:ASP:O	1:F:239:VAL:HG12	2.10	0.51
1:G:11:HIS:NE2	1:G:62:ARG:HD2	2.26	0.51
1:H:30:LEU:HD12	1:H:65:ARG:HG2	1.91	0.51
1:A:140:ARG:NH1	1:B:52:PHE:O	2.43	0.51
1:K:91:HIS:HD2	1:K:93:GLY:N	1.96	0.51
1:K:149:GLN:O	1:K:151:PRO:HD3	2.11	0.51
1:A:11:HIS:CE1	1:A:62:ARG:HD2	2.46	0.51
1:F:156:LEU:HD22	1:F:206:MET:HE3	1.90	0.51
1:L:160:ILE:HG12	1:L:192:GLY:CA	2.40	0.51
1:C:203:GLU:HA	1:C:206:MET:CE	2.41	0.51
1:A:158:ASP:O	1:A:161:ALA:HB3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:GLU:HA	1:C:206:MET:HE2	1.93	0.50
1:H:4:TYR:O	1:H:219:GLU:HA	2.10	0.50
1:J:53:ASP:OD1	1:J:180:ARG:NH1	2.44	0.50
1:K:227:ILE:HD12	1:K:227:ILE:O	2.11	0.50
1:L:23:SER:H	3:L:612:CIT:C5	2.24	0.50
1:A:29:ASP:OD2	1:A:65:ARG:NH1	2.44	0.50
1:B:72:ASP:OD2	1:B:77:MET:HE2	2.10	0.50
1:E:15:ALA:O	1:E:18:LEU:HD23	2.11	0.50
1:J:202:GLU:O	1:J:205:ILE:HG22	2.12	0.50
1:L:160:ILE:HG12	1:L:192:GLY:HA2	1.93	0.50
1:G:128:PRO:HA	1:G:133:TYR:CG	2.46	0.50
1:I:22:PHE:CE1	1:I:100:LYS:HG2	2.46	0.50
1:I:202:GLU:O	1:I:206:MET:HG3	2.11	0.50
1:C:11:HIS:CE1	1:C:62:ARG:HD2	2.46	0.50
1:I:51:GLU:HB2	1:I:180:ARG:NH2	2.27	0.50
1:A:43:GLN:HG3	1:A:46:ARG:NH2	2.25	0.50
1:B:180:ARG:HB3	4:B:630:HOH:O	2.10	0.50
1:J:240:ARG:HA	1:J:243:MET:CG	2.42	0.50
1:A:26:TYR:HA	1:A:136:ILE:CD1	2.42	0.50
1:B:128:PRO:HA	1:B:133:TYR:CG	2.46	0.50
1:E:128:PRO:HA	1:E:133:TYR:CG	2.47	0.50
1:I:72:ASP:OD1	1:J:65:ARG:NH2	2.44	0.50
1:J:26:TYR:HA	1:J:136:ILE:CD1	2.42	0.50
1:B:14:SER:H	1:B:17:ASN:ND2	2.02	0.50
1:C:72:ASP:OD1	1:D:65:ARG:NH2	2.45	0.50
1:F:128:PRO:HA	1:F:133:TYR:CG	2.47	0.50
1:G:51:GLU:HB2	1:G:180:ARG:HH21	1.77	0.50
1:J:91:HIS:HD2	1:J:93:GLY:N	1.97	0.50
1:K:116:ARG:NH2	4:K:625:HOH:O	2.45	0.50
1:L:91:HIS:HD2	1:L:93:GLY:N	1.96	0.50
1:A:62:ARG:NH1	4:A:612:HOH:O	2.44	0.50
1:A:172:VAL:HG13	1:A:224:LEU:HD11	1.93	0.50
1:B:167:TRP:O	1:B:172:VAL:HG23	2.12	0.50
1:C:12:GLY:HA2	1:C:212:THR:HB	1.92	0.50
1:D:160:ILE:HG12	1:D:192:GLY:HA2	1.94	0.50
1:D:161:ALA:O	1:D:165:PRO:HD3	2.12	0.50
1:F:117:ARG:HH21	1:F:207:GLU:CG	2.24	0.50
1:G:96:THR:O	1:G:130:HIS:CE1	2.65	0.50
1:H:29:ASP:OD2	1:H:65:ARG:NH1	2.45	0.50
1:K:11:HIS:CE1	1:K:62:ARG:HD2	2.46	0.50
1:L:85:TRP:O	1:L:88:ASN:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:TRP:O	1:B:88:ASN:HB2	2.10	0.49
1:H:23:SER:HB2	3:H:608:CIT:O4	2.12	0.49
1:H:172:VAL:HB	1:H:173:PRO:HD3	1.94	0.49
1:K:172:VAL:HB	1:K:173:PRO:HD3	1.94	0.49
1:F:72:ASP:OD2	1:F:77:MET:HE2	2.12	0.49
1:G:201:SER:O	1:G:204:ALA:HB3	2.12	0.49
1:H:228:LYS:HB2	1:H:229:PRO:HD2	1.93	0.49
1:L:128:PRO:HA	1:L:133:TYR:CG	2.48	0.49
1:C:109:GLU:OE1	1:C:109:GLU:HA	2.11	0.49
1:K:227:ILE:CD1	1:K:228:LYS:HE3	2.43	0.49
1:K:160:ILE:HG23	1:K:164:LEU:HD23	1.95	0.49
1:E:104:ALA:HA	1:E:112:VAL:HG21	1.94	0.49
1:F:164:LEU:CD2	1:F:164:LEU:N	2.75	0.49
1:F:202:GLU:O	1:F:205:ILE:HG22	2.13	0.49
1:G:52:PHE:O	1:H:140:ARG:NH1	2.45	0.49
1:K:164:LEU:HD11	1:K:196:HIS:HB2	1.94	0.49
1:B:36:GLU:HG3	1:B:40:ARG:NH1	2.28	0.49
1:C:128:PRO:HA	1:C:133:TYR:CG	2.47	0.49
1:C:172:VAL:HB	1:C:173:PRO:HD3	1.95	0.49
1:K:128:PRO:HA	1:K:133:TYR:CG	2.46	0.49
1:E:236:GLU:C	1:E:238:THR:N	2.66	0.49
1:I:200:LEU:HB3	1:I:204:ALA:HB3	1.93	0.49
1:L:215:PRO:HB2	1:L:233:LEU:HB2	1.94	0.49
1:A:3:ALA:HB3	1:A:220:LEU:O	2.12	0.49
1:B:90:ARG:HB2	1:B:159:THR:OG1	2.13	0.49
1:D:51:GLU:HB2	1:D:180:ARG:NH2	2.28	0.49
1:H:104:ALA:HA	1:H:112:VAL:HG21	1.94	0.49
1:I:172:VAL:HG13	1:I:224:LEU:CD1	2.41	0.49
1:E:80:PRO:HA	4:E:610:HOH:O	2.13	0.48
1:F:240:ARG:O	1:F:243:MET:HB2	2.12	0.48
1:G:111:GLN:HG3	1:G:115:TRP:CZ3	2.47	0.48
1:G:43:GLN:HE21	1:G:46:ARG:NH2	2.11	0.48
1:I:162:ARG:C	1:I:165:PRO:HD2	2.32	0.48
1:J:242:ALA:O	1:J:245:ALA:HB3	2.13	0.48
1:L:53:ASP:OD2	1:L:180:ARG:HD3	2.13	0.48
1:E:203:GLU:HA	1:E:206:MET:HE3	1.93	0.48
1:K:140:ARG:NH1	4:K:635:HOH:O	2.27	0.48
1:B:104:ALA:HA	1:B:112:VAL:HG21	1.95	0.48
1:D:72:ASP:OD2	1:D:77:MET:HE2	2.13	0.48
1:I:29:ASP:OD1	1:I:65:ARG:NH1	2.46	0.48
1:J:22:PHE:CZ	1:J:116:ARG:HD3	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:172:VAL:HB	1:J:173:PRO:HD3	1.95	0.48
1:L:87:LEU:O	1:L:186:HIS:HD2	1.95	0.48
1:D:104:ALA:HA	1:D:112:VAL:HG21	1.95	0.48
1:D:158:ASP:O	1:D:161:ALA:HB3	2.13	0.48
1:D:214:ILE:CD1	1:D:238:THR:HG22	2.44	0.48
1:I:23:SER:N	3:I:609:CIT:O4	2.45	0.48
1:I:164:LEU:HD12	1:I:168:ASN:ND2	2.28	0.48
1:J:128:PRO:HA	1:J:133:TYR:CG	2.48	0.48
1:B:224:LEU:N	1:B:224:LEU:HD23	2.28	0.48
1:D:172:VAL:HB	1:D:173:PRO:HD3	1.95	0.48
1:E:91:HIS:HD2	1:E:93:GLY:N	1.95	0.48
1:G:119:TYR:HB2	1:G:206:MET:CE	2.43	0.48
1:A:172:VAL:HB	1:A:173:PRO:HD3	1.95	0.48
1:B:36:GLU:HG3	1:B:40:ARG:HH12	1.79	0.48
1:D:2:ALA:HB2	1:D:219:GLU:OE1	2.14	0.48
1:D:29:ASP:OD2	1:D:65:ARG:NH1	2.47	0.48
1:I:120:ASP:HB3	1:I:157:LYS:HD2	1.95	0.48
1:I:160:ILE:HG12	1:I:192:GLY:HA2	1.95	0.48
1:L:100:LYS:NZ	3:L:612:CIT:H21	2.28	0.48
1:B:23:SER:HB2	3:B:602:CIT:O4	2.13	0.48
1:D:214:ILE:HD11	1:D:238:THR:HG22	1.95	0.48
1:E:29:ASP:OD2	1:E:65:ARG:NH1	2.47	0.48
1:I:219:GLU:HB3	4:I:626:HOH:O	2.13	0.48
1:L:243:MET:HA	1:L:243:MET:CE	2.40	0.48
1:C:166:PHE:CE1	1:C:170:GLU:HG3	2.48	0.48
1:E:166:PHE:CE1	1:E:170:GLU:HG3	2.48	0.48
1:F:172:VAL:HB	1:F:173:PRO:HD3	1.95	0.48
1:I:43:GLN:NE2	1:I:46:ARG:NH2	2.47	0.48
1:A:52:PHE:O	1:B:140:ARG:NH1	2.47	0.48
1:G:172:VAL:HB	1:G:173:PRO:HD3	1.95	0.48
1:H:195:LYS:CB	1:H:205:ILE:HD12	2.25	0.48
1:K:202:GLU:O	1:K:205:ILE:HG22	2.14	0.48
1:A:29:ASP:OD1	1:A:65:ARG:NH1	2.45	0.47
1:A:72:ASP:OD2	1:A:77:MET:HE2	2.14	0.47
1:F:164:LEU:N	1:F:164:LEU:HD22	2.28	0.47
1:G:140:ARG:NH1	1:H:52:PHE:O	2.47	0.47
1:I:172:VAL:HB	1:I:173:PRO:HD3	1.96	0.47
1:E:172:VAL:HB	1:E:173:PRO:HD3	1.95	0.47
1:H:90:ARG:NH2	1:H:115:TRP:O	2.46	0.47
1:L:51:GLU:HB2	1:L:180:ARG:HH21	1.78	0.47
1:B:172:VAL:HB	1:B:173:PRO:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ARG:NH2	1:D:72:ASP:OD1	2.47	0.47
1:D:128:PRO:HA	1:D:133:TYR:CG	2.49	0.47
1:F:142:TYR:HB3	1:F:145:LEU:HD12	1.96	0.47
1:K:160:ILE:HG23	1:K:164:LEU:CD2	2.44	0.47
1:A:160:ILE:HG23	1:A:164:LEU:CD2	2.44	0.47
1:H:128:PRO:HA	1:H:133:TYR:CG	2.49	0.47
1:A:51:GLU:HB2	1:A:180:ARG:HH21	1.77	0.47
1:B:12:GLY:HA2	1:B:212:THR:HB	1.96	0.47
1:E:43:GLN:CD	1:E:46:ARG:HH22	2.17	0.47
1:E:236:GLU:HA	1:E:240:ARG:H	1.78	0.47
1:J:22:PHE:HE1	1:J:116:ARG:HD3	1.75	0.47
1:A:128:PRO:HA	1:A:133:TYR:CG	2.49	0.47
1:I:195:LYS:HB2	1:I:205:ILE:CD1	2.44	0.47
1:G:164:LEU:HD11	1:G:196:HIS:CB	2.43	0.47
1:H:90:ARG:HB3	1:H:188:ASN:HD22	1.78	0.47
1:H:119:TYR:CE2	1:H:157:LYS:HB2	2.48	0.47
1:I:161:ALA:O	1:I:165:PRO:HD3	2.15	0.47
1:J:167:TRP:O	1:J:172:VAL:HG23	2.14	0.47
1:J:244:GLU:C	1:J:246:VAL:H	2.18	0.47
1:K:62:ARG:NH1	4:K:633:HOH:O	2.47	0.47
1:G:50:TYR:CE1	1:G:233:LEU:HD11	2.50	0.47
1:J:14:SER:H	1:J:17:ASN:ND2	2.03	0.47
1:A:160:ILE:O	1:A:164:LEU:HD23	2.15	0.47
1:H:53:ASP:OD2	1:H:180:ARG:HD3	2.15	0.47
1:I:119:TYR:HB2	1:I:206:MET:HE2	1.97	0.47
1:H:24:GLY:H	3:H:608:CIT:C5	2.27	0.47
1:J:29:ASP:OD2	1:J:65:ARG:NH1	2.48	0.47
1:K:227:ILE:O	1:K:228:LYS:HB3	2.14	0.47
1:L:26:TYR:HA	1:L:136:ILE:CD1	2.45	0.47
1:C:228:LYS:HB2	1:C:229:PRO:HD2	1.97	0.46
1:I:22:PHE:CZ	1:I:100:LYS:HG2	2.50	0.46
1:K:29:ASP:OD1	1:K:65:ARG:NH1	2.49	0.46
1:L:20:ASN:ND2	1:L:100:LYS:HD2	2.31	0.46
1:A:195:LYS:HD2	1:A:205:ILE:HG21	1.98	0.46
1:J:155:SER:N	1:J:158:ASP:HB2	2.30	0.46
1:D:12:GLY:HA2	1:D:212:THR:HB	1.98	0.46
1:H:72:ASP:OD2	1:H:77:MET:HE2	2.16	0.46
1:I:128:PRO:HA	1:I:133:TYR:CG	2.50	0.46
1:J:11:HIS:NE2	1:J:62:ARG:HD2	2.30	0.46
1:K:29:ASP:OD2	1:K:65:ARG:NH1	2.49	0.46
1:B:160:ILE:HG12	1:B:192:GLY:HA2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:LYS:HD2	1:G:205:ILE:HG21	1.96	0.46
1:J:4:TYR:N	1:J:4:TYR:CD2	2.82	0.46
1:J:72:ASP:OD2	1:J:77:MET:HE2	2.15	0.46
1:B:30:LEU:HD12	1:B:65:ARG:HG2	1.96	0.46
1:B:211:PRO:HG2	1:B:232:PHE:CE2	2.50	0.46
1:G:114:ILE:O	1:G:118:SER:HB3	2.16	0.46
1:K:3:ALA:HB3	1:K:220:LEU:O	2.16	0.46
1:K:51:GLU:HB2	1:K:180:ARG:NH2	2.31	0.46
1:C:156:LEU:O	1:C:160:ILE:HG13	2.14	0.46
1:F:146:THR:HG23	1:F:149:GLN:CD	2.35	0.46
1:H:60:GLN:HB3	4:H:621:HOH:O	2.14	0.46
1:I:174:GLN:OE1	1:I:179:LYS:HG3	2.16	0.46
1:I:89:GLU:OE1	1:I:188:ASN:HB2	2.16	0.46
1:J:50:TYR:CE1	1:J:233:LEU:HD11	2.50	0.46
1:K:140:ARG:CD	4:K:635:HOH:O	2.62	0.46
1:L:244:GLU:C	1:L:246:VAL:H	2.19	0.46
1:H:146:THR:O	1:H:149:GLN:N	2.49	0.46
1:H:160:ILE:HG12	1:H:192:GLY:CA	2.46	0.46
1:H:202:GLU:O	1:H:205:ILE:HG22	2.16	0.46
1:C:72:ASP:OD2	1:C:77:MET:HE2	2.16	0.45
1:E:236:GLU:HB2	1:E:240:ARG:CB	2.46	0.45
1:J:215:PRO:HB2	1:J:233:LEU:HB2	1.98	0.45
1:A:240:ARG:HA	1:A:243:MET:HB2	1.99	0.45
1:F:243:MET:HA	1:F:243:MET:HE2	1.98	0.45
1:H:175:ILE:HG21	1:H:224:LEU:HD22	1.97	0.45
1:I:119:TYR:HB2	1:I:206:MET:CE	2.47	0.45
1:L:11:HIS:CE1	1:L:62:ARG:HD2	2.51	0.45
1:D:23:SER:HB2	3:D:604:CIT:O4	2.16	0.45
1:D:161:ALA:O	1:D:165:PRO:CD	2.64	0.45
1:I:72:ASP:CG	1:J:65:ARG:HH22	2.20	0.45
1:K:100:LYS:HZ3	3:K:611:CIT:H21	1.79	0.45
1:C:104:ALA:O	1:C:108:GLY:N	2.49	0.45
1:B:160:ILE:HG12	1:B:192:GLY:CA	2.47	0.45
1:D:95:LEU:HA	1:D:98:LEU:HD12	1.98	0.45
1:H:220:LEU:HB3	1:H:224:LEU:HA	1.99	0.45
1:I:90:ARG:NH2	1:I:115:TRP:O	2.49	0.45
1:C:14:SER:H	1:C:17:ASN:ND2	2.04	0.45
1:C:145:LEU:HD22	1:C:149:GLN:HB3	1.98	0.45
1:C:202:GLU:O	1:C:206:MET:HG3	2.16	0.45
1:E:52:PHE:N	1:E:76:GLN:HE22	2.07	0.45
1:F:85:TRP:CE2	1:F:145:LEU:HD21	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:ILE:HG23	1:G:164:LEU:CD2	2.46	0.45
1:H:232:PHE:HB2	1:H:239:VAL:HG23	1.98	0.45
1:C:227:ILE:O	1:C:228:LYS:HB3	2.17	0.45
1:L:110:ALA:O	1:L:114:ILE:HG12	2.17	0.45
1:B:124:PRO:HA	1:B:125:PRO:HD3	1.90	0.44
1:D:114:ILE:O	1:D:118:SER:CB	2.65	0.44
1:I:210:LEU:HA	1:I:211:PRO:HD3	1.87	0.44
1:J:228:LYS:HB2	1:J:229:PRO:HD2	1.98	0.44
1:L:167:TRP:O	1:L:172:VAL:HG23	2.18	0.44
1:L:232:PHE:HE1	1:L:243:MET:HE3	1.82	0.44
1:A:160:ILE:HG23	1:A:164:LEU:HD23	1.99	0.44
1:D:92:TYR:N	4:D:605:HOH:O	2.39	0.44
1:I:195:LYS:HB2	1:I:205:ILE:HD13	1.98	0.44
1:D:156:LEU:HD21	1:D:191:ARG:HD3	1.98	0.44
1:G:14:SER:H	1:G:17:ASN:ND2	2.02	0.44
1:G:72:ASP:OD2	1:G:77:MET:HE2	2.17	0.44
1:H:26:TYR:HA	1:H:136:ILE:CD1	2.46	0.44
1:K:224:LEU:HD23	1:K:224:LEU:N	2.32	0.44
1:L:172:VAL:HB	1:L:173:PRO:HD3	1.98	0.44
1:C:30:LEU:HD12	1:C:65:ARG:HG2	1.99	0.44
1:F:167:TRP:O	1:F:172:VAL:HG23	2.18	0.44
1:G:100:LYS:NZ	3:G:607:CIT:H21	2.33	0.44
1:H:210:LEU:HA	1:H:211:PRO:HD3	1.87	0.44
1:B:235:ASP:OD1	1:B:237:GLU:HG3	2.17	0.44
1:D:83:ARG:HG3	4:D:626:HOH:O	2.17	0.44
1:I:215:PRO:HB2	1:I:233:LEU:HG	1.99	0.44
1:J:23:SER:H	3:J:610:CIT:C5	2.30	0.44
1:K:236:GLU:O	1:K:240:ARG:CB	2.65	0.44
1:B:205:ILE:HD12	1:B:205:ILE:HA	1.86	0.44
1:E:26:TYR:CA	1:E:136:ILE:HD11	2.44	0.44
1:A:100:LYS:NZ	3:A:601:CIT:H21	2.33	0.44
1:B:52:PHE:N	1:B:76:GLN:HE22	2.10	0.44
1:C:124:PRO:HA	1:C:125:PRO:HD3	1.90	0.44
1:C:162:ARG:O	1:C:165:PRO:HD2	2.17	0.44
1:G:210:LEU:HA	1:G:211:PRO:HD3	1.87	0.44
1:B:51:GLU:HB2	1:B:180:ARG:HH21	1.80	0.44
1:I:217:VAL:CG2	1:I:233:LEU:HD21	2.43	0.44
1:E:29:ASP:OD1	1:E:30:LEU:N	2.50	0.44
1:I:51:GLU:HB2	1:I:180:ARG:HH21	1.83	0.44
1:J:164:LEU:N	1:J:165:PRO:CD	2.81	0.44
1:A:214:ILE:HG21	1:A:232:PHE:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:ASP:OD1	1:F:30:LEU:N	2.50	0.43
1:J:4:TYR:N	1:J:4:TYR:HD2	2.16	0.43
1:A:103:THR:HG22	1:A:112:VAL:CG2	2.48	0.43
1:G:243:MET:HA	1:G:243:MET:CE	2.46	0.43
1:I:78:TRP:HA	1:J:64:ILE:CD1	2.48	0.43
1:K:43:GLN:HE21	1:K:46:ARG:NH2	2.16	0.43
1:K:95:LEU:HA	1:K:98:LEU:HD12	2.00	0.43
1:C:90:ARG:NH2	1:C:115:TRP:O	2.41	0.43
1:C:169:GLU:O	1:C:173:PRO:HG2	2.17	0.43
1:K:168:ASN:ND2	4:K:623:HOH:O	2.45	0.43
1:C:232:PHE:HB2	1:C:239:VAL:HG23	2.00	0.43
1:D:160:ILE:HG12	1:D:192:GLY:CA	2.48	0.43
1:F:51:GLU:HB2	1:F:180:ARG:HH21	1.84	0.43
1:G:26:TYR:CA	1:G:136:ILE:HD11	2.35	0.43
1:I:52:PHE:N	1:I:76:GLN:HE22	2.07	0.43
1:H:242:ALA:C	1:H:244:GLU:N	2.71	0.43
1:I:77:MET:HE1	1:J:65:ARG:NH2	2.33	0.43
1:B:228:LYS:HB2	1:B:229:PRO:HD2	2.01	0.43
1:C:29:ASP:OD1	1:C:30:LEU:N	2.52	0.43
1:C:72:ASP:CG	1:D:65:ARG:NH2	2.71	0.43
1:C:158:ASP:O	1:C:161:ALA:HB3	2.19	0.43
1:I:220:LEU:HB3	1:I:224:LEU:HA	2.00	0.43
1:H:7:VAL:HA	1:H:216:ILE:O	2.19	0.43
1:H:94:GLY:HA2	1:H:130:HIS:CD2	2.54	0.43
1:J:52:PHE:N	1:J:76:GLN:HE22	2.08	0.43
1:K:52:PHE:CD2	1:K:182:LEU:HB2	2.54	0.43
1:A:18:LEU:HD23	1:A:18:LEU:H	1.83	0.43
1:D:191:ARG:HH12	1:D:206:MET:HE1	1.84	0.43
1:E:14:SER:H	1:E:17:ASN:ND2	2.02	0.43
1:E:202:GLU:O	1:E:205:ILE:HG22	2.19	0.43
1:J:103:THR:O	1:J:107:HIS:HB2	2.18	0.43
1:K:160:ILE:CG2	1:K:164:LEU:HD23	2.49	0.43
1:E:51:GLU:HB2	1:E:180:ARG:HH21	1.84	0.43
1:G:11:HIS:CE1	1:G:62:ARG:HD2	2.53	0.43
1:G:108:GLY:C	1:G:110:ALA:N	2.71	0.43
1:I:14:SER:H	1:I:17:ASN:ND2	2.02	0.43
1:I:205:ILE:CG2	1:I:206:MET:N	2.81	0.43
1:K:164:LEU:N	1:K:165:PRO:CD	2.81	0.43
1:B:50:TYR:CE1	1:B:233:LEU:HD11	2.54	0.42
1:B:95:LEU:HA	1:B:98:LEU:HD12	2.00	0.42
1:B:138:LYS:HD3	1:B:138:LYS:HA	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:THR:HA	4:H:620:HOH:O	2.19	0.42
1:J:95:LEU:HA	1:J:98:LEU:HD12	2.01	0.42
1:A:81:VAL:HG13	1:B:83:ARG:NH1	2.34	0.42
1:D:160:ILE:CG2	1:D:164:LEU:HD22	2.49	0.42
1:E:95:LEU:HA	1:E:98:LEU:HD12	2.01	0.42
1:E:124:PRO:HA	1:E:125:PRO:HD3	1.90	0.42
1:E:138:LYS:HD3	1:E:138:LYS:HA	1.77	0.42
1:H:221:ASP:OD1	1:H:223:ASN:N	2.45	0.42
1:K:23:SER:N	3:K:611:CIT:O4	2.49	0.42
1:L:16:TRP:CZ3	1:L:97:GLY:HA2	2.54	0.42
1:F:18:LEU:HD23	1:F:18:LEU:H	1.84	0.42
1:G:166:PHE:CE1	1:G:170:GLU:HG3	2.53	0.42
1:H:95:LEU:HA	1:H:98:LEU:HD12	2.01	0.42
1:I:232:PHE:HE1	1:I:242:ALA:O	2.02	0.42
1:K:22:PHE:CZ	1:K:100:LYS:HG2	2.54	0.42
1:K:172:VAL:HG13	1:K:224:LEU:HD11	2.00	0.42
1:A:155:SER:O	1:A:156:LEU:C	2.58	0.42
1:D:11:HIS:CE1	1:D:62:ARG:HD2	2.54	0.42
1:D:156:LEU:HD22	1:D:191:ARG:NH1	2.34	0.42
1:J:141:ARG:HE	1:J:141:ARG:HB2	1.50	0.42
1:J:159:THR:HG23	1:J:162:ARG:CZ	2.49	0.42
1:L:90:ARG:HB3	1:L:188:ASN:ND2	2.34	0.42
1:C:51:GLU:HB2	1:C:180:ARG:HH21	1.84	0.42
1:G:209:ASN:HA	4:G:612:HOH:O	2.19	0.42
1:I:124:PRO:HA	1:I:125:PRO:HD3	1.89	0.42
1:J:4:TYR:CE1	1:J:175:ILE:HG22	2.54	0.42
1:J:11:HIS:CE1	1:J:62:ARG:HD2	2.54	0.42
1:J:236:GLU:HA	1:J:239:VAL:HG12	2.00	0.42
1:L:14:SER:H	1:L:17:ASN:ND2	2.05	0.42
1:D:85:TRP:NE1	1:D:145:LEU:HD21	2.35	0.42
1:G:83:ARG:NH1	1:H:81:VAL:HG13	2.34	0.42
1:G:217:VAL:CG2	1:G:233:LEU:HG	2.50	0.42
1:K:67:LEU:CD2	1:K:71:LEU:HG	2.49	0.42
1:A:191:ARG:O	1:A:205:ILE:HD11	2.19	0.42
1:C:14:SER:H	1:C:17:ASN:HB2	1.85	0.42
1:D:210:LEU:HA	1:D:211:PRO:HD3	1.87	0.42
1:E:52:PHE:CD2	1:E:182:LEU:HB2	2.54	0.42
1:E:72:ASP:OD2	1:E:77:MET:HE1	2.20	0.42
1:E:119:TYR:CE2	1:E:157:LYS:HG3	2.55	0.42
1:F:110:ALA:HB3	4:F:625:HOH:O	2.20	0.42
1:H:51:GLU:OE1	1:H:180:ARG:NH2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:ARG:HB3	1:H:205:ILE:HD11	2.02	0.42
1:L:220:LEU:HB3	1:L:224:LEU:HA	2.00	0.42
1:B:195:LYS:HB2	1:B:205:ILE:HG12	2.02	0.42
1:E:164:LEU:HD11	1:E:196:HIS:CG	2.55	0.42
1:F:172:VAL:HG13	1:F:224:LEU:CD1	2.42	0.42
1:L:195:LYS:HB2	1:L:205:ILE:HD13	2.02	0.42
1:B:14:SER:H	1:B:17:ASN:HB2	1.85	0.42
1:B:128:PRO:HA	1:B:133:TYR:CD1	2.55	0.42
1:F:124:PRO:HA	1:F:125:PRO:HD3	1.89	0.42
1:G:3:ALA:HB3	1:G:220:LEU:O	2.20	0.42
1:K:22:PHE:CE1	1:K:100:LYS:HG2	2.55	0.42
1:K:114:ILE:O	1:K:118:SER:HB3	2.19	0.42
1:L:10:ARG:NH1	1:L:210:LEU:O	2.52	0.42
1:A:55:CYS:SG	1:A:71:LEU:HD21	2.60	0.42
1:E:18:LEU:HD23	1:E:18:LEU:H	1.85	0.42
1:G:160:ILE:O	1:G:164:LEU:HD23	2.19	0.42
1:A:239:VAL:O	1:A:243:MET:N	2.52	0.41
1:H:117:ARG:O	1:H:118:SER:C	2.59	0.41
1:I:169:GLU:O	1:I:173:PRO:HG2	2.19	0.41
1:K:104:ALA:O	1:K:108:GLY:N	2.49	0.41
1:K:162:ARG:C	1:K:165:PRO:HD2	2.40	0.41
1:A:210:LEU:HA	1:A:211:PRO:HD3	1.86	0.41
1:H:67:LEU:CD2	1:H:71:LEU:HG	2.49	0.41
1:A:14:SER:H	1:A:17:ASN:ND2	2.01	0.41
1:A:133:TYR:CE2	1:A:138:LYS:HE2	2.55	0.41
1:A:221:ASP:OD2	1:A:225:LYS:HB3	2.19	0.41
1:C:140:ARG:NH1	1:D:52:PHE:O	2.52	0.41
1:F:221:ASP:CA	1:F:227:ILE:HD11	2.50	0.41
1:G:164:LEU:O	1:G:165:PRO:C	2.59	0.41
1:H:29:ASP:OD1	1:H:30:LEU:N	2.49	0.41
1:L:95:LEU:HA	1:L:98:LEU:HD12	2.01	0.41
1:L:128:PRO:HA	1:L:133:TYR:CD1	2.56	0.41
1:A:243:MET:HA	1:A:243:MET:HE2	2.02	0.41
1:C:128:PRO:HA	1:C:133:TYR:CD1	2.56	0.41
1:E:128:PRO:HA	1:E:133:TYR:CD1	2.55	0.41
1:E:228:LYS:HB2	1:E:229:PRO:HD2	2.02	0.41
1:F:128:PRO:HA	1:F:133:TYR:CD1	2.55	0.41
1:F:175:ILE:HG21	1:F:224:LEU:CD2	2.50	0.41
1:F:176:LYS:C	1:F:178:GLY:H	2.24	0.41
1:G:65:ARG:HH22	1:H:72:ASP:CG	2.24	0.41
1:H:52:PHE:O	1:H:79:LEU:HD21	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:221:ASP:C	1:I:223:ASN:H	2.23	0.41
1:J:203:GLU:HA	1:J:206:MET:HE2	2.01	0.41
1:J:244:GLU:C	1:J:246:VAL:N	2.72	0.41
1:K:164:LEU:HD11	1:K:196:HIS:CB	2.50	0.41
1:E:65:ARG:NH2	1:F:72:ASP:OD1	2.54	0.41
1:E:114:ILE:O	1:E:118:SER:HB3	2.19	0.41
1:E:220:LEU:HB3	1:E:224:LEU:HA	2.02	0.41
1:E:221:ASP:OD1	1:E:223:ASN:N	2.51	0.41
1:F:52:PHE:O	1:F:79:LEU:HD21	2.21	0.41
1:I:8:LEU:HB2	1:I:216:ILE:HB	2.02	0.41
1:I:29:ASP:OD1	1:I:30:LEU:N	2.52	0.41
1:F:95:LEU:HA	1:F:98:LEU:HD12	2.02	0.41
1:H:4:TYR:HB2	1:H:220:LEU:O	2.20	0.41
1:H:46:ARG:HG3	1:H:46:ARG:HH11	1.86	0.41
1:H:124:PRO:HA	1:H:125:PRO:HD3	1.93	0.41
1:I:85:TRP:CD1	1:I:145:LEU:HD21	2.55	0.41
1:J:20:ASN:ND2	1:J:100:LYS:HD2	2.34	0.41
1:G:65:ARG:NH2	1:H:72:ASP:CG	2.74	0.41
1:J:190:LEU:HD23	1:J:190:LEU:HA	1.90	0.41
1:J:228:LYS:HG3	1:J:229:PRO:O	2.20	0.41
1:K:128:PRO:HA	1:K:133:TYR:CD1	2.56	0.41
1:L:190:LEU:HD23	1:L:190:LEU:HA	1.93	0.41
1:L:239:VAL:O	1:L:240:ARG:C	2.58	0.41
1:C:220:LEU:HB3	1:C:224:LEU:HA	2.03	0.41
1:D:116:ARG:HD2	3:D:604:CIT:O1	2.20	0.41
1:G:95:LEU:HA	1:G:98:LEU:HD12	2.01	0.41
1:I:42:GLY:O	1:I:43:GLN:C	2.59	0.41
1:L:210:LEU:HA	1:L:211:PRO:HD3	1.87	0.41
1:A:111:GLN:NE2	1:A:115:TRP:CE2	2.89	0.41
1:A:239:VAL:O	1:A:243:MET:HB2	2.20	0.41
1:C:95:LEU:HA	1:C:98:LEU:HD12	2.02	0.41
1:F:4:TYR:CZ	1:F:176:LYS:HA	2.56	0.41
1:F:46:ARG:HH11	1:F:46:ARG:HG3	1.86	0.41
1:F:155:SER:N	1:F:158:ASP:HB2	2.34	0.41
1:F:159:THR:HG23	1:F:162:ARG:CZ	2.50	0.41
1:G:18:LEU:HD23	1:G:18:LEU:H	1.86	0.41
1:G:67:LEU:CD2	1:G:71:LEU:HG	2.48	0.41
1:G:128:PRO:HA	1:G:133:TYR:CD1	2.56	0.41
1:G:155:SER:N	1:G:158:ASP:OD2	2.45	0.41
1:G:228:LYS:HB2	1:G:229:PRO:HD2	2.03	0.41
1:H:18:LEU:HD23	1:H:18:LEU:H	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:29:ASP:OD1	1:K:30:LEU:N	2.51	0.41
1:K:231:GLN:O	1:K:232:PHE:HD2	2.03	0.41
1:A:95:LEU:HA	1:A:98:LEU:HD12	2.03	0.41
1:B:9:ILE:O	1:B:9:ILE:HG23	2.20	0.41
1:B:52:PHE:O	1:B:79:LEU:HD21	2.21	0.41
1:C:215:PRO:HB2	1:C:233:LEU:HB2	2.03	0.41
1:D:141:ARG:HE	1:D:141:ARG:HB2	1.53	0.41
1:G:155:SER:C	1:G:157:LYS:N	2.73	0.41
1:I:232:PHE:CE1	1:I:243:MET:HE3	2.56	0.41
1:K:18:LEU:HD23	1:K:18:LEU:H	1.84	0.41
1:K:160:ILE:HG12	1:K:192:GLY:CA	2.51	0.41
1:L:46:ARG:HG3	1:L:46:ARG:HH11	1.86	0.41
1:A:92:TYR:HE2	4:A:613:HOH:O	2.04	0.40
1:A:220:LEU:HB3	1:A:224:LEU:HA	2.02	0.40
1:B:237:GLU:HG3	1:B:238:THR:H	1.85	0.40
1:D:156:LEU:HD12	1:D:156:LEU:HA	1.89	0.40
1:G:52:PHE:N	1:G:76:GLN:HE22	2.08	0.40
1:L:93:GLY:HA2	1:L:152:SER:O	2.21	0.40
1:A:29:ASP:OD1	1:A:30:LEU:N	2.54	0.40
1:F:100:LYS:NZ	3:F:606:CIT:H21	2.36	0.40
1:G:177:GLU:HG2	1:J:40:ARG:NH2	2.30	0.40
1:H:6:LEU:HB3	1:H:218:TYR:HB2	2.03	0.40
1:H:190:LEU:HD23	1:H:190:LEU:HA	1.89	0.40
1:J:240:ARG:HA	1:J:243:MET:HG3	2.04	0.40
1:K:140:ARG:HH12	1:L:76:GLN:NE2	2.20	0.40
1:A:52:PHE:CD2	1:A:182:LEU:HB2	2.57	0.40
1:E:91:HIS:CD2	4:E:622:HOH:O	2.75	0.40
1:F:239:VAL:O	1:F:243:MET:HG2	2.21	0.40
1:H:38:ALA:O	1:H:42:GLY:N	2.54	0.40
1:I:81:VAL:HG13	1:J:83:ARG:NH1	2.37	0.40
1:I:190:LEU:HD23	1:I:190:LEU:HA	1.93	0.40
1:K:228:LYS:HB2	1:K:229:PRO:HD2	2.02	0.40
1:L:14:SER:H	1:L:17:ASN:HB2	1.86	0.40
1:A:83:ARG:NH1	1:B:81:VAL:HG13	2.36	0.40
1:D:18:LEU:HD23	1:D:18:LEU:H	1.85	0.40
1:E:20:ASN:ND2	1:E:100:LYS:HD2	2.36	0.40
1:G:190:LEU:HD23	1:G:190:LEU:HA	1.92	0.40
1:H:29:ASP:OD1	1:H:65:ARG:NH1	2.51	0.40
1:C:92:TYR:CE2	3:C:603:CIT:H22	2.56	0.40
1:E:51:GLU:OE1	1:E:180:ARG:NH2	2.55	0.40
1:G:16:TRP:CZ3	1:G:97:GLY:HA2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:168:ASN:O	1:G:173:PRO:HD3	2.22	0.40
1:H:155:SER:N	1:H:158:ASP:HB2	2.35	0.40
1:I:205:ILE:HD12	1:I:205:ILE:HA	1.93	0.40
1:L:214:ILE:HA	1:L:215:PRO:HD3	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	243/262 (93%)	223 (92%)	19 (8%)	1 (0%)	34 66
1	B	240/262 (92%)	220 (92%)	20 (8%)	0	100 100
1	C	241/262 (92%)	221 (92%)	20 (8%)	0	100 100
1	D	243/262 (93%)	226 (93%)	15 (6%)	2 (1%)	19 49
1	E	241/262 (92%)	224 (93%)	17 (7%)	0	100 100
1	F	240/262 (92%)	221 (92%)	19 (8%)	0	100 100
1	G	243/262 (93%)	221 (91%)	18 (7%)	4 (2%)	9 31
1	H	239/262 (91%)	221 (92%)	16 (7%)	2 (1%)	19 49
1	I	240/262 (92%)	222 (92%)	17 (7%)	1 (0%)	34 66
1	J	242/262 (92%)	227 (94%)	15 (6%)	0	100 100
1	K	237/262 (90%)	225 (95%)	10 (4%)	2 (1%)	19 49
1	L	243/262 (93%)	224 (92%)	18 (7%)	1 (0%)	34 66
All	All	2892/3144 (92%)	2675 (92%)	204 (7%)	13 (0%)	34 66

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	235	ASP
1	D	243	MET
1	G	110	ALA
1	G	146	THR
1	K	235	ASP
1	A	224	LEU
1	D	236	GLU
1	G	236	GLU
1	H	243	MET
1	K	222	LYS
1	L	240	ARG
1	H	118	SER
1	G	205	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/220 (88%)	185 (95%)	9 (5%)	27	60
1	B	195/220 (89%)	187 (96%)	8 (4%)	30	64
1	C	193/220 (88%)	184 (95%)	9 (5%)	26	59
1	D	194/220 (88%)	185 (95%)	9 (5%)	27	60
1	E	192/220 (87%)	185 (96%)	7 (4%)	35	69
1	F	192/220 (87%)	183 (95%)	9 (5%)	26	59
1	G	188/220 (86%)	178 (95%)	10 (5%)	22	54
1	H	190/220 (86%)	181 (95%)	9 (5%)	26	59
1	I	196/220 (89%)	188 (96%)	8 (4%)	30	64
1	J	196/220 (89%)	186 (95%)	10 (5%)	24	55
1	K	189/220 (86%)	183 (97%)	6 (3%)	39	73
1	L	195/220 (89%)	186 (95%)	9 (5%)	27	60
All	All	2314/2640 (88%)	2211 (96%)	103 (4%)	27	60

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	18	LEU
1	A	43	GLN
1	A	62	ARG
1	A	67	LEU
1	A	81	VAL
1	A	90	ARG
1	A	92	TYR
1	A	243	MET
1	B	6	LEU
1	B	18	LEU
1	B	62	ARG
1	B	67	LEU
1	B	81	VAL
1	B	90	ARG
1	B	92	TYR
1	B	224	LEU
1	C	6	LEU
1	C	18	LEU
1	C	43	GLN
1	C	62	ARG
1	C	67	LEU
1	C	90	ARG
1	C	92	TYR
1	C	118	SER
1	C	223	ASN
1	D	6	LEU
1	D	18	LEU
1	D	43	GLN
1	D	62	ARG
1	D	67	LEU
1	D	81	VAL
1	D	90	ARG
1	D	92	TYR
1	D	164	LEU
1	E	6	LEU
1	E	62	ARG
1	E	67	LEU
1	E	81	VAL
1	E	90	ARG
1	E	92	TYR
1	E	164	LEU
1	F	6	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	18	LEU
1	F	62	ARG
1	F	67	LEU
1	F	81	VAL
1	F	90	ARG
1	F	92	TYR
1	F	177	GLU
1	F	238	THR
1	G	6	LEU
1	G	18	LEU
1	G	62	ARG
1	G	67	LEU
1	G	81	VAL
1	G	90	ARG
1	G	92	TYR
1	G	112	VAL
1	G	239	VAL
1	G	243	MET
1	H	6	LEU
1	H	18	LEU
1	H	43	GLN
1	H	62	ARG
1	H	67	LEU
1	H	81	VAL
1	H	90	ARG
1	H	92	TYR
1	H	227	ILE
1	I	6	LEU
1	I	62	ARG
1	I	67	LEU
1	I	81	VAL
1	I	90	ARG
1	I	92	TYR
1	I	112	VAL
1	I	164	LEU
1	J	4	TYR
1	J	6	LEU
1	J	18	LEU
1	J	43	GLN
1	J	62	ARG
1	J	67	LEU
1	J	81	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	90	ARG
1	J	92	TYR
1	J	145	LEU
1	K	6	LEU
1	K	18	LEU
1	K	67	LEU
1	K	81	VAL
1	K	90	ARG
1	K	92	TYR
1	L	6	LEU
1	L	18	LEU
1	L	43	GLN
1	L	62	ARG
1	L	67	LEU
1	L	81	VAL
1	L	90	ARG
1	L	92	TYR
1	L	243	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	20	ASN
1	A	76	GLN
1	A	91	HIS
1	A	188	ASN
1	B	17	ASN
1	B	20	ASN
1	B	76	GLN
1	B	91	HIS
1	C	17	ASN
1	C	20	ASN
1	C	76	GLN
1	C	91	HIS
1	C	223	ASN
1	D	17	ASN
1	D	20	ASN
1	D	76	GLN
1	D	91	HIS
1	E	17	ASN
1	E	20	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	76	GLN
1	E	91	HIS
1	E	111	GLN
1	F	17	ASN
1	F	20	ASN
1	F	76	GLN
1	F	91	HIS
1	F	188	ASN
1	G	17	ASN
1	G	20	ASN
1	G	43	GLN
1	G	76	GLN
1	G	91	HIS
1	G	107	HIS
1	H	17	ASN
1	H	20	ASN
1	H	43	GLN
1	H	76	GLN
1	H	91	HIS
1	H	188	ASN
1	I	17	ASN
1	I	20	ASN
1	I	43	GLN
1	I	76	GLN
1	I	91	HIS
1	I	168	ASN
1	J	17	ASN
1	J	20	ASN
1	J	76	GLN
1	J	91	HIS
1	K	17	ASN
1	K	20	ASN
1	K	43	GLN
1	K	76	GLN
1	K	91	HIS
1	K	168	ASN
1	L	17	ASN
1	L	20	ASN
1	L	76	GLN
1	L	91	HIS
1	L	188	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CIT	F	606	-	12,12,12	1.97	4 (33%)	17,17,17	3.23	10 (58%)
3	CIT	I	609	-	12,12,12	2.10	2 (16%)	17,17,17	3.26	10 (58%)
3	CIT	B	602	-	12,12,12	2.08	3 (25%)	17,17,17	3.28	10 (58%)
3	CIT	A	601	-	12,12,12	2.36	3 (25%)	17,17,17	3.19	7 (41%)
3	CIT	H	608	-	12,12,12	2.22	4 (33%)	17,17,17	3.12	9 (52%)
3	CIT	G	607	-	12,12,12	2.56	4 (33%)	17,17,17	3.07	7 (41%)
3	CIT	E	605	-	12,12,12	2.47	5 (41%)	17,17,17	3.00	9 (52%)
3	CIT	K	611	-	12,12,12	2.12	3 (25%)	17,17,17	3.23	10 (58%)
3	CIT	C	603	-	12,12,12	2.09	4 (33%)	17,17,17	3.34	10 (58%)
3	CIT	J	610	-	12,12,12	2.44	4 (33%)	17,17,17	2.79	7 (41%)
3	CIT	D	604	-	12,12,12	2.44	4 (33%)	17,17,17	2.69	9 (52%)
3	CIT	L	612	-	12,12,12	2.48	4 (33%)	17,17,17	3.03	8 (47%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIT	F	606	-	-	6/16/16/16	-
3	CIT	I	609	-	-	7/16/16/16	-
3	CIT	B	602	-	-	9/16/16/16	-
3	CIT	A	601	-	-	4/16/16/16	-
3	CIT	H	608	-	-	9/16/16/16	-
3	CIT	G	607	-	-	5/16/16/16	-
3	CIT	E	605	-	-	6/16/16/16	-
3	CIT	K	611	-	-	5/16/16/16	-
3	CIT	C	603	-	-	9/16/16/16	-
3	CIT	J	610	-	-	9/16/16/16	-
3	CIT	D	604	-	-	5/16/16/16	-
3	CIT	L	612	-	-	4/16/16/16	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	612	CIT	C3-C6	6.08	1.59	1.53
3	G	607	CIT	C3-C6	5.91	1.59	1.53
3	H	608	CIT	C3-C6	5.71	1.59	1.53
3	J	610	CIT	C3-C6	5.65	1.59	1.53
3	D	604	CIT	C3-C6	5.60	1.59	1.53
3	E	605	CIT	C3-C6	5.41	1.59	1.53
3	A	601	CIT	C3-C6	5.40	1.59	1.53
3	I	609	CIT	C3-C6	5.23	1.58	1.53
3	K	611	CIT	C3-C6	4.95	1.58	1.53
3	B	602	CIT	C3-C6	4.83	1.58	1.53
3	C	603	CIT	C3-C6	4.55	1.58	1.53
3	G	607	CIT	C4-C3	4.08	1.58	1.53
3	E	605	CIT	C4-C3	4.03	1.58	1.53
3	D	604	CIT	C4-C3	4.00	1.58	1.53
3	J	610	CIT	C4-C3	3.93	1.58	1.53
3	A	601	CIT	C4-C3	3.92	1.58	1.53
3	L	612	CIT	C4-C3	3.87	1.58	1.53
3	F	606	CIT	C3-C6	3.72	1.57	1.53
3	C	603	CIT	O2-C1	-3.52	1.18	1.30
3	G	607	CIT	O2-C1	-3.49	1.19	1.30
3	L	612	CIT	O2-C1	-3.47	1.19	1.30
3	J	610	CIT	O2-C1	-3.46	1.19	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	609	CIT	O2-C1	-3.43	1.19	1.30
3	D	604	CIT	O2-C1	-3.42	1.19	1.30
3	E	605	CIT	O2-C1	-3.40	1.19	1.30
3	K	611	CIT	O2-C1	-3.38	1.19	1.30
3	F	606	CIT	O2-C1	-3.36	1.19	1.30
3	A	601	CIT	O2-C1	-3.32	1.19	1.30
3	H	608	CIT	O2-C1	-3.26	1.19	1.30
3	B	602	CIT	O2-C1	-3.22	1.19	1.30
3	F	606	CIT	C4-C3	3.11	1.57	1.53
3	K	611	CIT	C4-C3	2.91	1.57	1.53
3	B	602	CIT	C4-C3	2.63	1.57	1.53
3	H	608	CIT	C4-C3	2.54	1.57	1.53
3	D	604	CIT	C4-C5	2.49	1.58	1.50
3	C	603	CIT	C2-C3	2.48	1.56	1.53
3	G	607	CIT	C4-C5	2.46	1.58	1.50
3	L	612	CIT	C4-C5	2.28	1.57	1.50
3	E	605	CIT	C4-C5	2.25	1.57	1.50
3	E	605	CIT	C2-C3	2.22	1.56	1.53
3	J	610	CIT	C4-C5	2.21	1.57	1.50
3	C	603	CIT	C4-C3	2.10	1.56	1.53
3	F	606	CIT	C4-C5	2.02	1.56	1.50
3	H	608	CIT	O1-C1	2.01	1.28	1.22

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	CIT	O7-C3-C6	-7.18	98.79	108.86
3	B	602	CIT	C2-C3-C6	6.79	124.70	110.11
3	H	608	CIT	C2-C3-C6	6.62	124.34	110.11
3	L	612	CIT	O7-C3-C6	-6.60	99.60	108.86
3	C	603	CIT	C2-C3-C6	6.32	123.68	110.11
3	A	601	CIT	C2-C3-C6	6.31	123.65	110.11
3	I	609	CIT	C2-C3-C6	6.14	123.31	110.11
3	B	602	CIT	O7-C3-C6	-6.07	100.34	108.86
3	K	611	CIT	C2-C3-C6	6.03	123.07	110.11
3	F	606	CIT	C2-C3-C6	6.00	123.00	110.11
3	F	606	CIT	O7-C3-C6	-5.99	100.46	108.86
3	G	607	CIT	C2-C3-C6	5.87	122.72	110.11
3	K	611	CIT	O6-C6-C3	-5.81	102.95	113.05
3	F	606	CIT	O6-C6-C3	-5.81	102.96	113.05
3	C	603	CIT	O6-C6-C3	-5.80	102.98	113.05
3	G	607	CIT	O7-C3-C6	-5.76	100.78	108.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	605	CIT	C2-C3-C6	5.73	122.42	110.11
3	I	609	CIT	O6-C6-C3	-5.71	103.14	113.05
3	C	603	CIT	O5-C6-C3	5.66	130.27	122.25
3	I	609	CIT	O7-C3-C6	-5.66	100.92	108.86
3	K	611	CIT	O7-C3-C6	-5.65	100.94	108.86
3	I	609	CIT	O5-C6-C3	5.63	130.23	122.25
3	K	611	CIT	O5-C6-C3	5.63	130.22	122.25
3	G	607	CIT	O6-C6-C3	-5.58	103.37	113.05
3	C	603	CIT	O7-C3-C6	-5.57	101.04	108.86
3	G	607	CIT	O5-C6-C3	5.57	130.14	122.25
3	F	606	CIT	O5-C6-C3	5.46	129.98	122.25
3	E	605	CIT	O6-C6-C3	-5.43	103.61	113.05
3	L	612	CIT	O6-C6-C3	-5.40	103.67	113.05
3	E	605	CIT	O5-C6-C3	5.38	129.87	122.25
3	B	602	CIT	O6-C6-C3	-5.38	103.70	113.05
3	L	612	CIT	C2-C3-C6	5.36	121.63	110.11
3	B	602	CIT	O5-C6-C3	5.36	129.84	122.25
3	A	601	CIT	O6-C6-C3	-5.27	103.90	113.05
3	L	612	CIT	O5-C6-C3	5.24	129.68	122.25
3	J	610	CIT	O5-C6-C3	5.21	129.63	122.25
3	E	605	CIT	O7-C3-C6	-5.09	101.71	108.86
3	D	604	CIT	C2-C3-C6	5.07	121.01	110.11
3	J	610	CIT	O6-C6-C3	-5.07	104.24	113.05
3	H	608	CIT	O6-C6-C3	-5.02	104.34	113.05
3	A	601	CIT	O5-C6-C3	5.01	129.35	122.25
3	H	608	CIT	O7-C3-C6	-4.98	101.88	108.86
3	D	604	CIT	O5-C6-C3	4.94	129.25	122.25
3	J	610	CIT	C2-C3-C6	4.93	120.70	110.11
3	H	608	CIT	O5-C6-C3	4.92	129.22	122.25
3	J	610	CIT	O7-C3-C6	-4.67	102.30	108.86
3	D	604	CIT	O6-C6-C3	-4.60	105.05	113.05
3	C	603	CIT	C4-C3-C6	-4.46	100.53	110.11
3	H	608	CIT	C4-C3-C6	-4.29	100.88	110.11
3	I	609	CIT	C4-C3-C6	-4.20	101.08	110.11
3	D	604	CIT	O7-C3-C6	-4.01	103.24	108.86
3	B	602	CIT	C4-C3-C6	-3.97	101.58	110.11
3	F	606	CIT	C4-C3-C6	-3.72	102.11	110.11
3	K	611	CIT	C4-C3-C6	-3.66	102.24	110.11
3	D	604	CIT	C4-C3-C6	-3.40	102.80	110.11
3	J	610	CIT	C4-C3-C6	-3.22	103.18	110.11
3	C	603	CIT	C3-C4-C5	-3.10	106.30	113.81
3	E	605	CIT	C4-C3-C6	-2.90	103.87	110.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	607	CIT	C4-C3-C6	-2.82	104.04	110.11
3	E	605	CIT	O2-C1-C2	2.76	123.23	114.35
3	K	611	CIT	O2-C1-C2	2.70	123.01	114.35
3	H	608	CIT	O2-C1-C2	2.66	122.90	114.35
3	A	601	CIT	O2-C1-C2	2.60	122.70	114.35
3	L	612	CIT	O2-C1-C2	2.59	122.67	114.35
3	I	609	CIT	O2-C1-C2	2.58	122.65	114.35
3	G	607	CIT	O2-C1-C2	2.58	122.64	114.35
3	J	610	CIT	O2-C1-C2	2.57	122.60	114.35
3	F	606	CIT	O2-C1-C2	2.54	122.51	114.35
3	D	604	CIT	O2-C1-C2	2.52	122.44	114.35
3	B	602	CIT	O2-C1-C2	2.51	122.43	114.35
3	D	604	CIT	O3-C5-C4	2.49	130.22	122.94
3	C	603	CIT	O2-C1-C2	2.46	122.25	114.35
3	H	608	CIT	C3-C4-C5	-2.39	108.02	113.81
3	H	608	CIT	O1-C1-C2	-2.38	115.99	122.94
3	I	609	CIT	C3-C4-C5	-2.32	108.19	113.81
3	E	605	CIT	O1-C1-C2	-2.32	116.17	122.94
3	K	611	CIT	O4-C5-C4	-2.29	107.01	114.35
3	C	603	CIT	O4-C5-C4	-2.28	107.01	114.35
3	K	611	CIT	C3-C4-C5	-2.26	108.34	113.81
3	K	611	CIT	O1-C1-C2	-2.25	116.37	122.94
3	F	606	CIT	C3-C4-C5	-2.25	108.37	113.81
3	B	602	CIT	O1-C1-C2	-2.25	116.38	122.94
3	D	604	CIT	O4-C5-C4	-2.21	107.27	114.35
3	D	604	CIT	O1-C1-C2	-2.17	116.59	122.94
3	A	601	CIT	O1-C1-C2	-2.17	116.60	122.94
3	B	602	CIT	O3-C5-C4	2.16	129.27	122.94
3	I	609	CIT	O1-C1-C2	-2.16	116.63	122.94
3	I	609	CIT	O4-C5-C4	-2.14	107.48	114.35
3	B	602	CIT	O4-C5-C4	-2.11	107.57	114.35
3	C	603	CIT	O3-C5-C4	2.11	129.11	122.94
3	G	607	CIT	O1-C1-C2	-2.11	116.78	122.94
3	L	612	CIT	O3-C5-C4	2.11	129.09	122.94
3	L	612	CIT	O1-C1-C2	-2.11	116.79	122.94
3	F	606	CIT	O1-C1-C2	-2.11	116.79	122.94
3	C	603	CIT	O1-C1-C2	-2.10	116.80	122.94
3	H	608	CIT	O4-C5-C4	-2.10	107.60	114.35
3	E	605	CIT	O4-C5-C4	-2.09	107.64	114.35
3	K	611	CIT	O3-C5-C4	2.09	129.04	122.94
3	I	609	CIT	O3-C5-C4	2.08	129.01	122.94
3	A	601	CIT	O4-C5-C4	-2.07	107.69	114.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	605	CIT	O3-C5-C4	2.07	128.98	122.94
3	L	612	CIT	O4-C5-C4	-2.06	107.73	114.35
3	F	606	CIT	O4-C5-C4	-2.04	107.79	114.35
3	B	602	CIT	C3-C4-C5	-2.04	108.87	113.81
3	J	610	CIT	O1-C1-C2	-2.02	117.05	122.94
3	F	606	CIT	O3-C5-C4	2.02	128.83	122.94

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	CIT	C2-C3-C4-C5
3	B	602	CIT	O7-C3-C4-C5
3	B	602	CIT	C2-C3-C6-O5
3	B	602	CIT	C2-C3-C6-O6
3	B	602	CIT	O7-C3-C6-O5
3	B	602	CIT	O7-C3-C6-O6
3	C	603	CIT	C2-C3-C6-O5
3	C	603	CIT	C2-C3-C6-O6
3	D	604	CIT	C2-C3-C4-C5
3	D	604	CIT	O7-C3-C4-C5
3	D	604	CIT	C6-C3-C4-C5
3	E	605	CIT	O7-C3-C6-O5
3	E	605	CIT	O7-C3-C6-O6
3	E	605	CIT	C4-C3-C6-O5
3	E	605	CIT	C4-C3-C6-O6
3	F	606	CIT	C6-C3-C4-C5
3	H	608	CIT	C2-C3-C4-C5
3	H	608	CIT	O7-C3-C4-C5
3	H	608	CIT	C6-C3-C4-C5
3	H	608	CIT	O7-C3-C6-O5
3	H	608	CIT	O7-C3-C6-O6
3	H	608	CIT	C4-C3-C6-O5
3	H	608	CIT	C4-C3-C6-O6
3	I	609	CIT	C6-C3-C4-C5
3	J	610	CIT	C6-C3-C4-C5
3	J	610	CIT	C2-C3-C6-O5
3	J	610	CIT	C2-C3-C6-O6
3	J	610	CIT	O7-C3-C6-O5
3	J	610	CIT	O7-C3-C6-O6
3	K	611	CIT	C6-C3-C4-C5
3	K	611	CIT	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	601	CIT	O7-C3-C4-C5
3	J	610	CIT	C2-C3-C4-C5
3	L	612	CIT	O7-C3-C4-C5
3	A	601	CIT	C2-C3-C4-C5
3	B	602	CIT	C6-C3-C4-C5
3	L	612	CIT	C2-C3-C4-C5
3	B	602	CIT	O1-C1-C2-C3
3	D	604	CIT	O1-C1-C2-C3
3	G	607	CIT	O1-C1-C2-C3
3	A	601	CIT	O1-C1-C2-C3
3	B	602	CIT	O2-C1-C2-C3
3	D	604	CIT	O2-C1-C2-C3
3	E	605	CIT	O1-C1-C2-C3
3	E	605	CIT	O2-C1-C2-C3
3	F	606	CIT	O1-C1-C2-C3
3	G	607	CIT	O2-C1-C2-C3
3	H	608	CIT	O1-C1-C2-C3
3	J	610	CIT	O1-C1-C2-C3
3	K	611	CIT	O1-C1-C2-C3
3	L	612	CIT	O1-C1-C2-C3
3	L	612	CIT	O2-C1-C2-C3
3	A	601	CIT	O2-C1-C2-C3
3	C	603	CIT	O1-C1-C2-C3
3	F	606	CIT	O2-C1-C2-C3
3	H	608	CIT	O2-C1-C2-C3
3	I	609	CIT	O1-C1-C2-C3
3	J	610	CIT	O2-C1-C2-C3
3	K	611	CIT	O2-C1-C2-C3
3	G	607	CIT	C2-C3-C4-C5
3	G	607	CIT	O7-C3-C4-C5
3	I	609	CIT	C2-C3-C4-C5
3	C	603	CIT	O7-C3-C6-O6
3	C	603	CIT	C4-C3-C6-O5
3	C	603	CIT	C4-C3-C6-O6
3	K	611	CIT	O7-C3-C4-C5
3	C	603	CIT	O2-C1-C2-C3
3	I	609	CIT	O2-C1-C2-C3
3	F	606	CIT	C4-C3-C6-O6
3	I	609	CIT	C4-C3-C6-O6
3	F	606	CIT	C2-C3-C4-C5
3	J	610	CIT	O7-C3-C4-C5
3	C	603	CIT	O7-C3-C6-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	F	606	CIT	C4-C3-C6-O5
3	G	607	CIT	C4-C3-C6-O6
3	I	609	CIT	C4-C3-C6-O5
3	C	603	CIT	C6-C3-C4-C5
3	I	609	CIT	C2-C3-C6-O6

There are no ring outliers.

11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	606	CIT	1	0
3	I	609	CIT	1	0
3	B	602	CIT	2	0
3	A	601	CIT	1	0
3	H	608	CIT	2	0
3	G	607	CIT	1	0
3	K	611	CIT	3	0
3	C	603	CIT	1	0
3	J	610	CIT	2	0
3	D	604	CIT	2	0
3	L	612	CIT	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	245/262 (93%)	-0.32	3 (1%) 79 73	19, 33, 55, 81	0
1	B	242/262 (92%)	-0.30	3 (1%) 79 73	18, 33, 49, 78	0
1	C	243/262 (92%)	-0.23	0 100 100	18, 34, 51, 84	0
1	D	245/262 (93%)	-0.27	1 (0%) 92 91	18, 36, 54, 74	0
1	E	243/262 (92%)	-0.13	2 (0%) 86 81	21, 36, 56, 88	0
1	F	242/262 (92%)	-0.21	3 (1%) 79 73	20, 36, 56, 95	0
1	G	245/262 (93%)	-0.14	3 (1%) 79 73	21, 38, 61, 85	0
1	H	241/262 (91%)	-0.21	2 (0%) 86 81	21, 37, 53, 90	0
1	I	242/262 (92%)	-0.06	2 (0%) 86 81	20, 37, 60, 91	0
1	J	244/262 (93%)	-0.19	0 100 100	20, 38, 58, 91	0
1	K	239/262 (91%)	-0.22	4 (1%) 70 63	19, 35, 49, 102	0
1	L	245/262 (93%)	-0.18	0 100 100	18, 32, 52, 82	0
All	All	2916/3144 (92%)	-0.20	23 (0%) 86 81	18, 35, 57, 102	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	234	GLY	4.1
1	K	235	ASP	3.4
1	G	104	ALA	3.4
1	F	244	GLU	3.0
1	A	2	ALA	2.7
1	K	240	ARG	2.7
1	D	104	ALA	2.6
1	E	2	ALA	2.6
1	B	2	ALA	2.5
1	H	242	ALA	2.4
1	F	178	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	239	VAL	2.4
1	B	237	GLU	2.3
1	A	235	ASP	2.3
1	G	148	ASP	2.3
1	I	46	ARG	2.3
1	G	135	ASN	2.3
1	A	19	GLU	2.2
1	E	19	GLU	2.2
1	I	235	ASP	2.1
1	H	244	GLU	2.1
1	B	242	ALA	2.1
1	K	236	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CIT	G	607	13/13	0.77	0.30	72,74,77,77	0
3	CIT	H	608	13/13	0.80	0.38	72,74,81,81	0
3	CIT	F	606	13/13	0.84	0.35	73,76,81,82	0
3	CIT	J	610	13/13	0.85	0.27	64,65,69,71	0
3	CIT	D	604	13/13	0.86	0.28	65,67,70,71	0
3	CIT	E	605	13/13	0.86	0.27	69,71,72,72	0
3	CIT	C	603	13/13	0.86	0.25	55,57,59,59	0
3	CIT	K	611	13/13	0.86	0.33	61,62,63,64	0
3	CIT	B	602	13/13	0.87	0.32	69,70,73,74	0
3	CIT	I	609	13/13	0.87	0.27	55,56,58,58	0
3	CIT	L	612	13/13	0.90	0.23	49,52,55,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CIT	A	601	13/13	0.92	0.25	48,50,55,58	0
2	CL	F	263	1/1	0.97	0.14	31,31,31,31	0
2	CL	H	263	1/1	0.97	0.09	25,25,25,25	0
2	CL	K	263	1/1	0.97	0.14	21,21,21,21	0
2	CL	C	263	1/1	0.99	0.18	23,23,23,23	0
2	CL	J	263	1/1	0.99	0.09	32,32,32,32	0
2	CL	A	263	1/1	0.99	0.08	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.