Full wwPDB X-ray Structure Validation Report (i)

Sep 22, 2020 – 04:11 PM EDT

PDB ID	:	6WA6
Title	:	Structure of the Chlamydia pneumoniae CdsV protein
Authors	:	Jensen, J.L.; Spiller, B.W.
Deposited on	:	2020-03-24
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 following versions of software and data (see references (1)) were used in the production of this report:

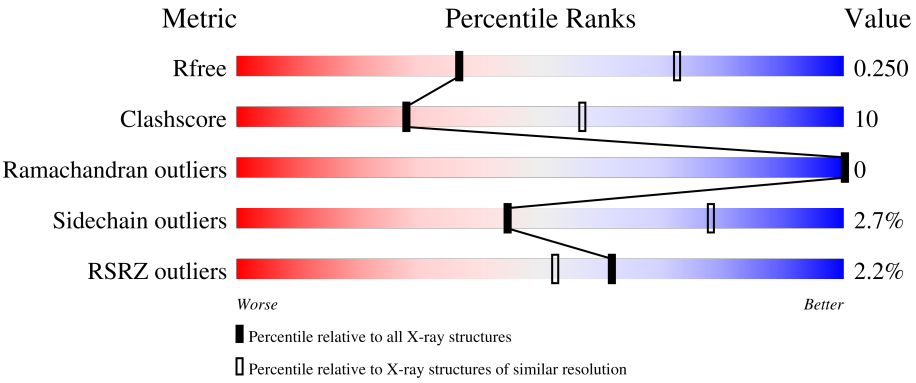
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 on 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	387	73% 16% • 10%
1	B	387	67% 21% • 10%
1	C	387	69% 19% 12%
1	D	387	74% 14% 11%
1	E	387	67% 21% • 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	387	2% 65% 22% 12%
1	G	387	2% 72% 16% 11%
1	H	387	4% 61% 21% 17%
1	I	387	3% 68% 18% 14%

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
2	GOL	B	802	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24992 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 Low calcium response locus protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	5	0
			2845	1843	470	525	7			
1	B	347	Total	C	N	O	S	0	0	0
			2800	1811	461	521	7			
1	C	342	Total	C	N	O	S	0	0	0
			2767	1790	457	513	7			
1	D	343	Total	C	N	O	S	0	2	0
			2793	1808	461	517	7			
1	E	343	Total	C	N	O	S	0	0	0
			2779	1798	457	517	7			
1	F	340	Total	C	N	O	S	0	1	0
			2755	1783	453	512	7			
1	G	343	Total	C	N	O	S	0	1	0
			2773	1794	455	517	7			
1	H	320	Total	C	N	O	S	0	0	0
			2609	1692	425	485	7			
1	I	334	Total	C	N	O	S	0	3	0
			2735	1770	452	506	7			

There are 189 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	MET	-	initiating methionine	UNP Q9Z8L5
A	325	GLY	-	expression tag	UNP Q9Z8L5
A	326	SER	-	expression tag	UNP Q9Z8L5
A	327	SER	-	expression tag	UNP Q9Z8L5
A	328	HIS	-	expression tag	UNP Q9Z8L5
A	329	HIS	-	expression tag	UNP Q9Z8L5
A	330	HIS	-	expression tag	UNP Q9Z8L5
A	331	HIS	-	expression tag	UNP Q9Z8L5
A	332	HIS	-	expression tag	UNP Q9Z8L5
A	333	HIS	-	expression tag	UNP Q9Z8L5
A	334	SER	-	expression tag	UNP Q9Z8L5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	SER	-	expression tag	UNP Q9Z8L5
A	336	GLY	-	expression tag	UNP Q9Z8L5
A	337	LEU	-	expression tag	UNP Q9Z8L5
A	338	VAL	-	expression tag	UNP Q9Z8L5
A	339	PRO	-	expression tag	UNP Q9Z8L5
A	340	ARG	-	expression tag	UNP Q9Z8L5
A	341	GLY	-	expression tag	UNP Q9Z8L5
A	342	SER	-	expression tag	UNP Q9Z8L5
A	343	HIS	-	expression tag	UNP Q9Z8L5
A	344	MET	-	expression tag	UNP Q9Z8L5
B	324	MET	-	initiating methionine	UNP Q9Z8L5
B	325	GLY	-	expression tag	UNP Q9Z8L5
B	326	SER	-	expression tag	UNP Q9Z8L5
B	327	SER	-	expression tag	UNP Q9Z8L5
B	328	HIS	-	expression tag	UNP Q9Z8L5
B	329	HIS	-	expression tag	UNP Q9Z8L5
B	330	HIS	-	expression tag	UNP Q9Z8L5
B	331	HIS	-	expression tag	UNP Q9Z8L5
B	332	HIS	-	expression tag	UNP Q9Z8L5
B	333	HIS	-	expression tag	UNP Q9Z8L5
B	334	SER	-	expression tag	UNP Q9Z8L5
B	335	SER	-	expression tag	UNP Q9Z8L5
B	336	GLY	-	expression tag	UNP Q9Z8L5
B	337	LEU	-	expression tag	UNP Q9Z8L5
B	338	VAL	-	expression tag	UNP Q9Z8L5
B	339	PRO	-	expression tag	UNP Q9Z8L5
B	340	ARG	-	expression tag	UNP Q9Z8L5
B	341	GLY	-	expression tag	UNP Q9Z8L5
B	342	SER	-	expression tag	UNP Q9Z8L5
B	343	HIS	-	expression tag	UNP Q9Z8L5
B	344	MET	-	expression tag	UNP Q9Z8L5
C	324	MET	-	initiating methionine	UNP Q9Z8L5
C	325	GLY	-	expression tag	UNP Q9Z8L5
C	326	SER	-	expression tag	UNP Q9Z8L5
C	327	SER	-	expression tag	UNP Q9Z8L5
C	328	HIS	-	expression tag	UNP Q9Z8L5
C	329	HIS	-	expression tag	UNP Q9Z8L5
C	330	HIS	-	expression tag	UNP Q9Z8L5
C	331	HIS	-	expression tag	UNP Q9Z8L5
C	332	HIS	-	expression tag	UNP Q9Z8L5
C	333	HIS	-	expression tag	UNP Q9Z8L5
C	334	SER	-	expression tag	UNP Q9Z8L5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	335	SER	-	expression tag	UNP Q9Z8L5
C	336	GLY	-	expression tag	UNP Q9Z8L5
C	337	LEU	-	expression tag	UNP Q9Z8L5
C	338	VAL	-	expression tag	UNP Q9Z8L5
C	339	PRO	-	expression tag	UNP Q9Z8L5
C	340	ARG	-	expression tag	UNP Q9Z8L5
C	341	GLY	-	expression tag	UNP Q9Z8L5
C	342	SER	-	expression tag	UNP Q9Z8L5
C	343	HIS	-	expression tag	UNP Q9Z8L5
C	344	MET	-	expression tag	UNP Q9Z8L5
D	324	MET	-	initiating methionine	UNP Q9Z8L5
D	325	GLY	-	expression tag	UNP Q9Z8L5
D	326	SER	-	expression tag	UNP Q9Z8L5
D	327	SER	-	expression tag	UNP Q9Z8L5
D	328	HIS	-	expression tag	UNP Q9Z8L5
D	329	HIS	-	expression tag	UNP Q9Z8L5
D	330	HIS	-	expression tag	UNP Q9Z8L5
D	331	HIS	-	expression tag	UNP Q9Z8L5
D	332	HIS	-	expression tag	UNP Q9Z8L5
D	333	HIS	-	expression tag	UNP Q9Z8L5
D	334	SER	-	expression tag	UNP Q9Z8L5
D	335	SER	-	expression tag	UNP Q9Z8L5
D	336	GLY	-	expression tag	UNP Q9Z8L5
D	337	LEU	-	expression tag	UNP Q9Z8L5
D	338	VAL	-	expression tag	UNP Q9Z8L5
D	339	PRO	-	expression tag	UNP Q9Z8L5
D	340	ARG	-	expression tag	UNP Q9Z8L5
D	341	GLY	-	expression tag	UNP Q9Z8L5
D	342	SER	-	expression tag	UNP Q9Z8L5
D	343	HIS	-	expression tag	UNP Q9Z8L5
D	344	MET	-	expression tag	UNP Q9Z8L5
E	324	MET	-	initiating methionine	UNP Q9Z8L5
E	325	GLY	-	expression tag	UNP Q9Z8L5
E	326	SER	-	expression tag	UNP Q9Z8L5
E	327	SER	-	expression tag	UNP Q9Z8L5
E	328	HIS	-	expression tag	UNP Q9Z8L5
E	329	HIS	-	expression tag	UNP Q9Z8L5
E	330	HIS	-	expression tag	UNP Q9Z8L5
E	331	HIS	-	expression tag	UNP Q9Z8L5
E	332	HIS	-	expression tag	UNP Q9Z8L5
E	333	HIS	-	expression tag	UNP Q9Z8L5
E	334	SER	-	expression tag	UNP Q9Z8L5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	335	SER	-	expression tag	UNP Q9Z8L5
E	336	GLY	-	expression tag	UNP Q9Z8L5
E	337	LEU	-	expression tag	UNP Q9Z8L5
E	338	VAL	-	expression tag	UNP Q9Z8L5
E	339	PRO	-	expression tag	UNP Q9Z8L5
E	340	ARG	-	expression tag	UNP Q9Z8L5
E	341	GLY	-	expression tag	UNP Q9Z8L5
E	342	SER	-	expression tag	UNP Q9Z8L5
E	343	HIS	-	expression tag	UNP Q9Z8L5
E	344	MET	-	expression tag	UNP Q9Z8L5
F	324	MET	-	initiating methionine	UNP Q9Z8L5
F	325	GLY	-	expression tag	UNP Q9Z8L5
F	326	SER	-	expression tag	UNP Q9Z8L5
F	327	SER	-	expression tag	UNP Q9Z8L5
F	328	HIS	-	expression tag	UNP Q9Z8L5
F	329	HIS	-	expression tag	UNP Q9Z8L5
F	330	HIS	-	expression tag	UNP Q9Z8L5
F	331	HIS	-	expression tag	UNP Q9Z8L5
F	332	HIS	-	expression tag	UNP Q9Z8L5
F	333	HIS	-	expression tag	UNP Q9Z8L5
F	334	SER	-	expression tag	UNP Q9Z8L5
F	335	SER	-	expression tag	UNP Q9Z8L5
F	336	GLY	-	expression tag	UNP Q9Z8L5
F	337	LEU	-	expression tag	UNP Q9Z8L5
F	338	VAL	-	expression tag	UNP Q9Z8L5
F	339	PRO	-	expression tag	UNP Q9Z8L5
F	340	ARG	-	expression tag	UNP Q9Z8L5
F	341	GLY	-	expression tag	UNP Q9Z8L5
F	342	SER	-	expression tag	UNP Q9Z8L5
F	343	HIS	-	expression tag	UNP Q9Z8L5
F	344	MET	-	expression tag	UNP Q9Z8L5
G	324	MET	-	initiating methionine	UNP Q9Z8L5
G	325	GLY	-	expression tag	UNP Q9Z8L5
G	326	SER	-	expression tag	UNP Q9Z8L5
G	327	SER	-	expression tag	UNP Q9Z8L5
G	328	HIS	-	expression tag	UNP Q9Z8L5
G	329	HIS	-	expression tag	UNP Q9Z8L5
G	330	HIS	-	expression tag	UNP Q9Z8L5
G	331	HIS	-	expression tag	UNP Q9Z8L5
G	332	HIS	-	expression tag	UNP Q9Z8L5
G	333	HIS	-	expression tag	UNP Q9Z8L5
G	334	SER	-	expression tag	UNP Q9Z8L5

Continued on next page...

Continued from previous page...

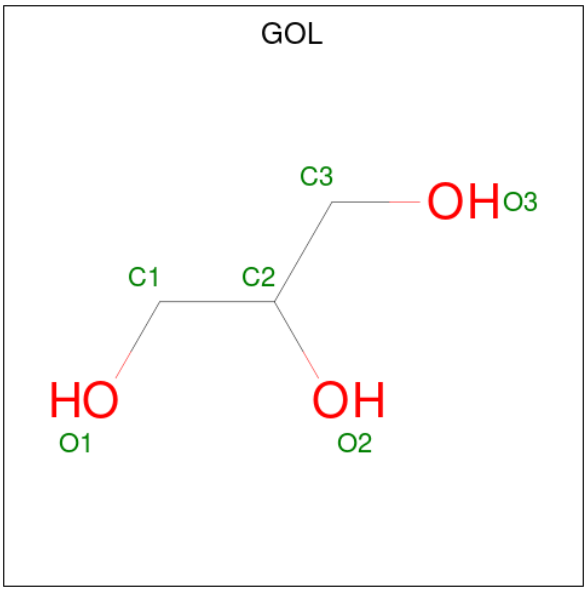
Chain	Residue	Modelled	Actual	Comment	Reference
G	335	SER	-	expression tag	UNP Q9Z8L5
G	336	GLY	-	expression tag	UNP Q9Z8L5
G	337	LEU	-	expression tag	UNP Q9Z8L5
G	338	VAL	-	expression tag	UNP Q9Z8L5
G	339	PRO	-	expression tag	UNP Q9Z8L5
G	340	ARG	-	expression tag	UNP Q9Z8L5
G	341	GLY	-	expression tag	UNP Q9Z8L5
G	342	SER	-	expression tag	UNP Q9Z8L5
G	343	HIS	-	expression tag	UNP Q9Z8L5
G	344	MET	-	expression tag	UNP Q9Z8L5
H	324	MET	-	initiating methionine	UNP Q9Z8L5
H	325	GLY	-	expression tag	UNP Q9Z8L5
H	326	SER	-	expression tag	UNP Q9Z8L5
H	327	SER	-	expression tag	UNP Q9Z8L5
H	328	HIS	-	expression tag	UNP Q9Z8L5
H	329	HIS	-	expression tag	UNP Q9Z8L5
H	330	HIS	-	expression tag	UNP Q9Z8L5
H	331	HIS	-	expression tag	UNP Q9Z8L5
H	332	HIS	-	expression tag	UNP Q9Z8L5
H	333	HIS	-	expression tag	UNP Q9Z8L5
H	334	SER	-	expression tag	UNP Q9Z8L5
H	335	SER	-	expression tag	UNP Q9Z8L5
H	336	GLY	-	expression tag	UNP Q9Z8L5
H	337	LEU	-	expression tag	UNP Q9Z8L5
H	338	VAL	-	expression tag	UNP Q9Z8L5
H	339	PRO	-	expression tag	UNP Q9Z8L5
H	340	ARG	-	expression tag	UNP Q9Z8L5
H	341	GLY	-	expression tag	UNP Q9Z8L5
H	342	SER	-	expression tag	UNP Q9Z8L5
H	343	HIS	-	expression tag	UNP Q9Z8L5
H	344	MET	-	expression tag	UNP Q9Z8L5
I	324	MET	-	initiating methionine	UNP Q9Z8L5
I	325	GLY	-	expression tag	UNP Q9Z8L5
I	326	SER	-	expression tag	UNP Q9Z8L5
I	327	SER	-	expression tag	UNP Q9Z8L5
I	328	HIS	-	expression tag	UNP Q9Z8L5
I	329	HIS	-	expression tag	UNP Q9Z8L5
I	330	HIS	-	expression tag	UNP Q9Z8L5
I	331	HIS	-	expression tag	UNP Q9Z8L5
I	332	HIS	-	expression tag	UNP Q9Z8L5
I	333	HIS	-	expression tag	UNP Q9Z8L5
I	334	SER	-	expression tag	UNP Q9Z8L5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	335	SER	-	expression tag	UNP Q9Z8L5
I	336	GLY	-	expression tag	UNP Q9Z8L5
I	337	LEU	-	expression tag	UNP Q9Z8L5
I	338	VAL	-	expression tag	UNP Q9Z8L5
I	339	PRO	-	expression tag	UNP Q9Z8L5
I	340	ARG	-	expression tag	UNP Q9Z8L5
I	341	GLY	-	expression tag	UNP Q9Z8L5
I	342	SER	-	expression tag	UNP Q9Z8L5
I	343	HIS	-	expression tag	UNP Q9Z8L5
I	344	MET	-	expression tag	UNP Q9Z8L5

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0
2	I	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

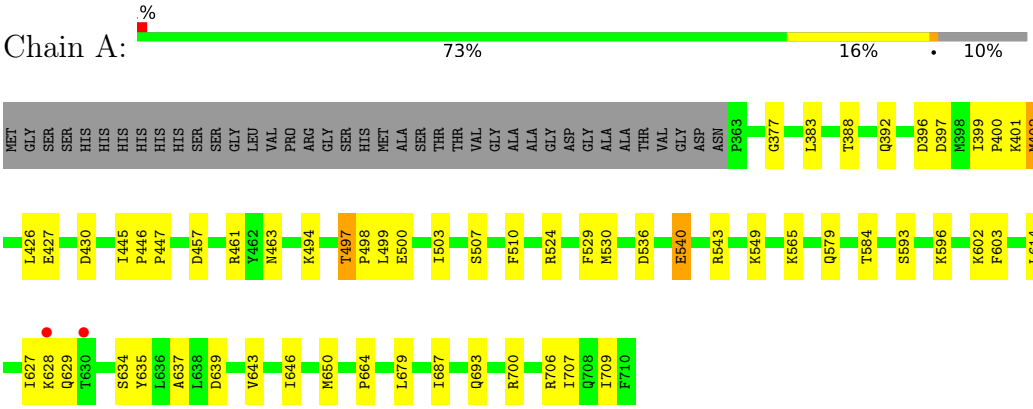
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	17	Total O 17 17	0	0
3	B	6	Total O 6 6	0	0
3	C	5	Total O 5 5	0	0
3	D	9	Total O 9 9	0	0
3	E	3	Total O 3 3	0	0
3	F	4	Total O 4 4	0	0
3	G	4	Total O 4 4	0	0
3	H	4	Total O 4 4	0	0
3	I	6	Total O 6 6	0	0

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.

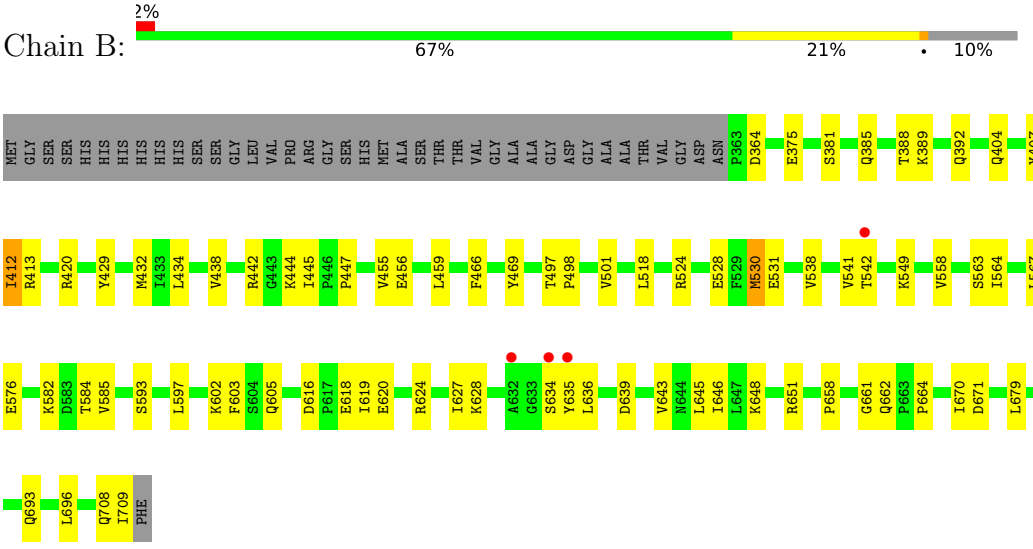
• Molecule 1: Low calcium response locus protein D

Chain A:



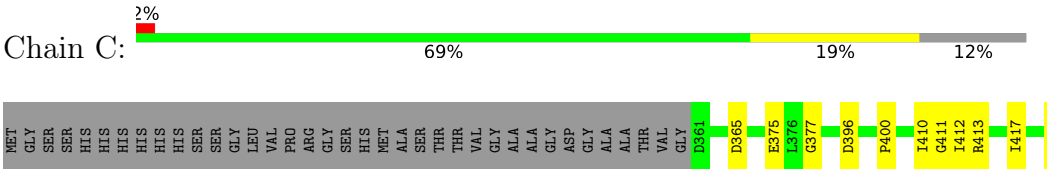
• Molecule 1: Low calcium response locus protein D

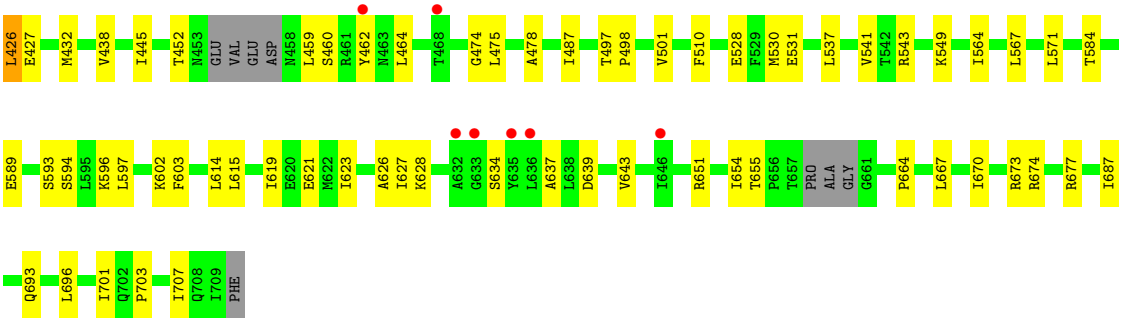
Chain B:



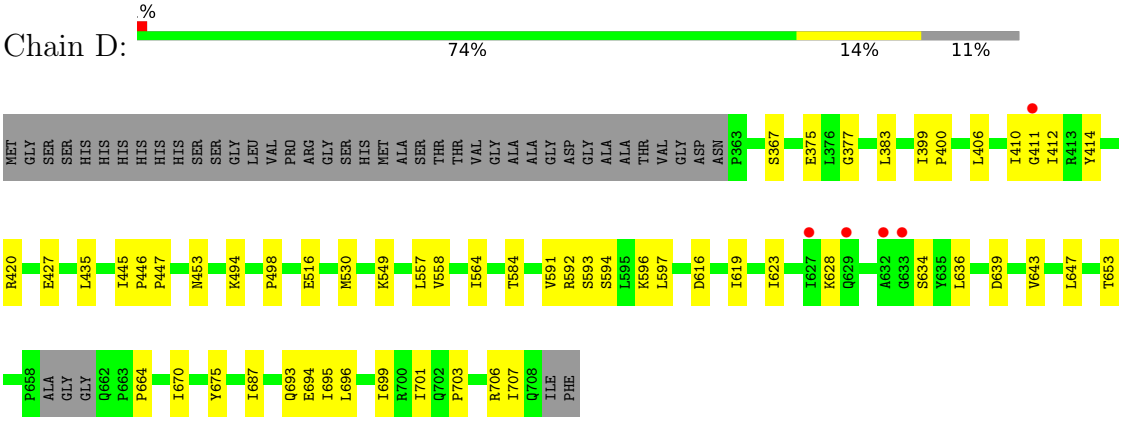
• Molecule 1: Low calcium response locus protein D

Chain C:

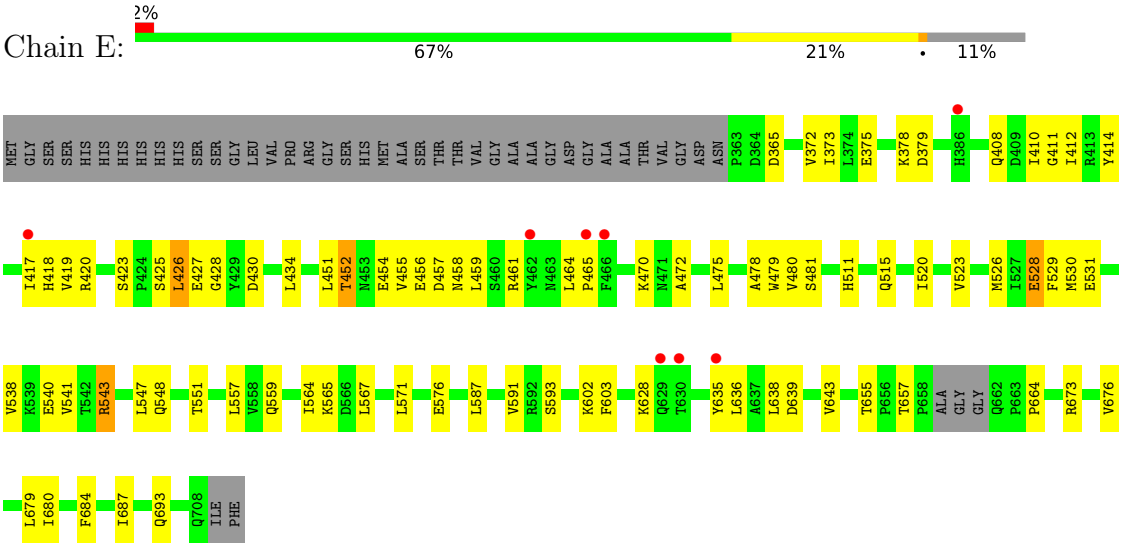




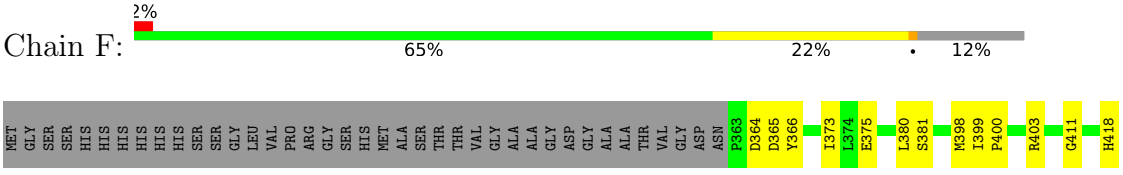
• Molecule 1: Low calcium response locus protein D

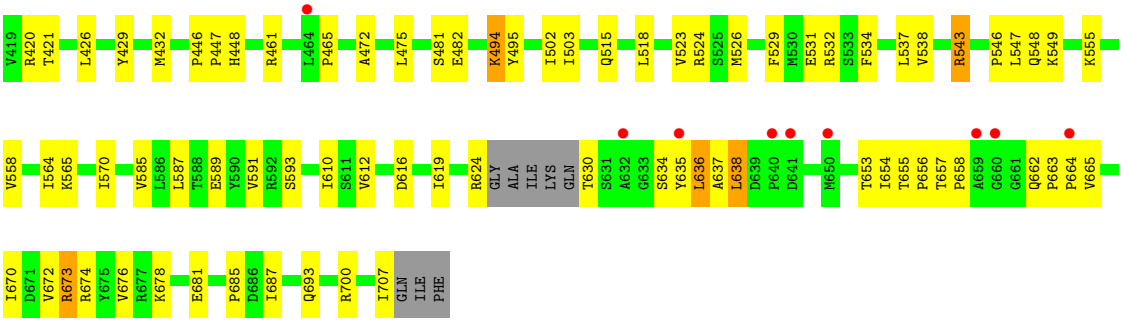


• Molecule 1: Low calcium response locus protein D



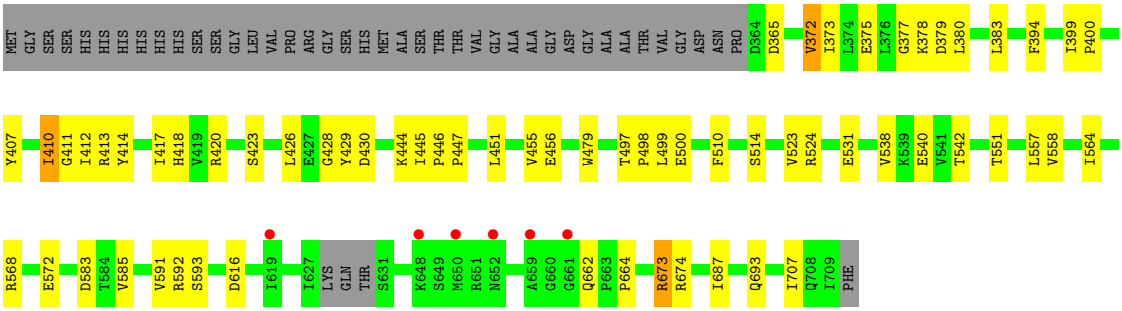
• Molecule 1: Low calcium response locus protein D





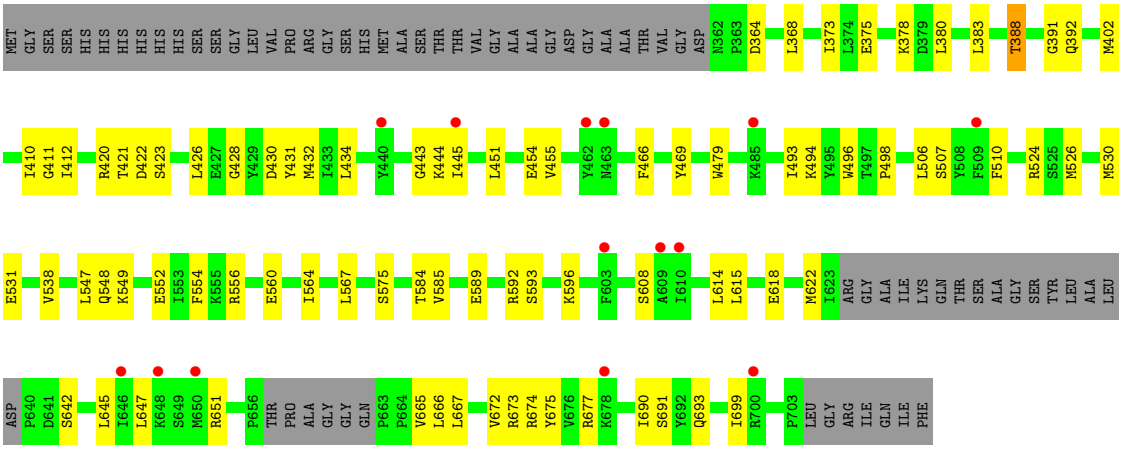
• Molecule 1: Low calcium response locus protein D

Chain G:



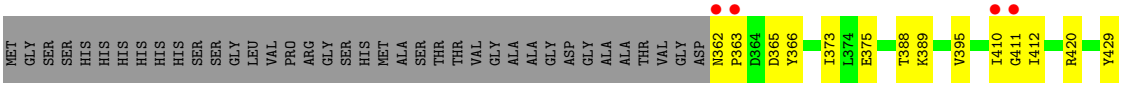
• Molecule 1: Low calcium response locus protein D

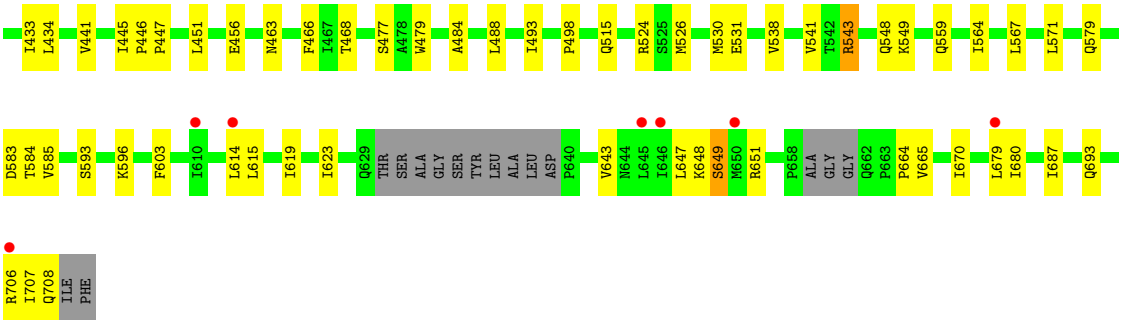
Chain H:



• Molecule 1: Low calcium response locus protein D

Chain I:




I433 L434 V441 I445 P446 P447 L451 E456 N463 F466 I467 T468 S477 A478 W479 A484 L488 I493 P498 Q515 R524 S525 M526 M530 E531 V538 V541 T542 R543 Q548 K549 Q559 I564 L567 L571 Q579
D583 T584 V585 S593 K596 F603 I610 L614 L615 I619 I623 Q629 THR SER ALA GLY SER TYR LEU ALA LEU ASP P640 V643 N644 L645 I646 L647 K648 S649 M650 R651 P658 ALA GLY GLY Q662 P663 P664 V665 I670 L679 I680 I687 Q693
R706 I707 Q708 ILE PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.65Å 280.44Å 290.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	126.27 – 2.80 126.27 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (126.27-2.80) 99.4 (126.27-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.196 , 0.244 0.207 , 0.250	Depositor DCC
R_{free} test set	6708 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	66.1	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24992	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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: GOL

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	0.54	0/2923	0.66	0/3965
1	B	0.46	0/2860	0.65	0/3881
1	C	0.41	0/2824	0.62	0/3829
1	D	0.43	0/2860	0.61	0/3880
1	E	0.46	0/2838	0.65	0/3850
1	F	0.44	0/2818	0.58	0/3824
1	G	0.44	0/2834	0.61	0/3845
1	H	0.43	0/2665	0.62	0/3614
1	I	0.45	0/2802	0.62	0/3799
All	All	0.45	0/25424	0.62	0/34487

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	2845	0	2930	41	0
1	B	2800	0	2880	57	0
1	C	2767	0	2847	48	0
1	D	2793	0	2871	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2779	0	2857	76	0
1	F	2755	0	2827	81	0
1	G	2773	0	2847	64	0
1	H	2609	0	2677	50	0
1	I	2735	0	2814	58	0
2	A	24	0	32	1	0
2	B	12	0	16	1	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	18	0	24	1	0
2	G	6	0	8	0	0
2	I	6	0	8	0	0
3	A	17	0	0	0	0
3	B	6	0	0	0	0
3	C	5	0	0	0	0
3	D	9	0	0	0	0
3	E	3	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	6	0	0	1	0
All	All	24992	0	25654	500	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 10.

All (500) 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:G:377:GLY:HA2	1:G:426:LEU:CD2	1.47	1.44
1:G:377:GLY:CA	1:G:426:LEU:HD22	1.52	1.38
1:E:464:LEU:CD1	1:E:465:PRO:HD3	1.54	1.33
1:G:412:ILE:HD11	1:G:558:VAL:CG2	1.69	1.20
1:E:464:LEU:HD12	1:E:465:PRO:CD	1.72	1.19
1:E:464:LEU:HD12	1:E:465:PRO:N	1.61	1.15
1:E:464:LEU:CG	1:E:465:PRO:HD3	1.80	1.12
1:G:412:ILE:HD12	1:G:514:SER:HB2	1.19	1.12
1:E:464:LEU:CD1	1:E:465:PRO:CD	2.26	1.11
1:F:546:PRO:HD2	1:F:549:LYS:HD2	1.20	1.11
1:G:412:ILE:CD1	1:G:558:VAL:HG21	1.82	1.09
1:F:612:VAL:HG12	1:F:665:VAL:HG11	1.15	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:653:THR:HG23	1:F:654:ILE:HD12	1.27	1.07
1:F:411:GLY:HA3	1:F:564:ILE:HG12	1.33	1.07
1:E:411:GLY:HA3	1:E:564:ILE:CG1	1.85	1.04
1:A:388:THR:OG1	1:A:392:GLN:HG2	1.61	1.00
1:C:628:LYS:HG3	1:C:634:SER:OG	1.62	0.99
1:F:612:VAL:CG1	1:F:665:VAL:HG11	1.93	0.99
1:E:464:LEU:HG	1:E:465:PRO:HD3	1.42	0.98
1:F:664:PRO:HG2	1:F:687:ILE:HA	1.44	0.97
1:C:541:VAL:HG11	1:C:571:LEU:HD22	1.49	0.94
1:B:624:ARG:HD3	1:B:671:ASP:OD2	1.67	0.94
1:E:411:GLY:HA3	1:E:564:ILE:HG13	1.47	0.94
1:F:653:THR:CG2	1:F:654:ILE:HD12	1.97	0.94
1:I:649:SER:HB3	1:I:707:ILE:HB	1.49	0.93
1:F:366:TYR:HD2	1:G:407:TYR:HH	1.15	0.93
1:I:614:LEU:CD1	1:I:706:ARG:HH21	1.81	0.92
1:F:546:PRO:CD	1:F:549:LYS:HD2	2.00	0.92
1:E:411:GLY:HA3	1:E:564:ILE:HG12	1.52	0.90
1:D:549:LYS:HE2	1:D:584:THR:HG22	1.54	0.89
1:F:399:ILE:O	1:F:403:ARG:HG3	1.74	0.88
1:I:362:ASN:N	1:I:363:PRO:CD	2.36	0.88
1:H:647:LEU:HB3	1:H:651:ARG:HH12	1.38	0.88
1:G:426:LEU:CD1	1:G:428:GLY:H	1.87	0.88
1:G:412:ILE:HD11	1:G:558:VAL:HG21	0.89	0.87
1:I:614:LEU:HD13	1:I:706:ARG:HH21	1.37	0.87
1:F:670:ILE:HD12	1:F:693:GLN:HB2	1.59	0.84
1:E:464:LEU:HG	1:E:465:PRO:CD	2.08	0.84
1:F:411:GLY:HA3	1:F:564:ILE:CG1	2.08	0.84
1:B:531:GLU:HG3	1:B:538:VAL:HG11	1.60	0.83
1:F:612:VAL:HG12	1:F:665:VAL:CG1	2.04	0.83
1:G:412:ILE:CD1	1:G:514:SER:HB2	2.07	0.83
1:I:541:VAL:HG11	1:I:571:LEU:HD22	1.60	0.82
1:E:464:LEU:CG	1:E:465:PRO:CD	2.57	0.82
1:E:464:LEU:HD11	1:E:465:PRO:HD3	1.60	0.82
1:I:614:LEU:HD13	1:I:706:ARG:NH2	1.95	0.81
1:F:657:THR:HG21	1:F:662:GLN:O	1.81	0.81
1:H:647:LEU:HB3	1:H:651:ARG:NH1	1.95	0.81
1:A:497:THR:HG22	1:A:500:GLU:H	1.46	0.80
1:I:614:LEU:HB2	1:I:706:ARG:HG2	1.64	0.80
1:I:410:ILE:HG21	1:I:412:ILE:HD12	1.64	0.80
1:B:645:LEU:HB3	1:B:709:ILE:HD13	1.64	0.78
1:B:388:THR:HG22	1:B:389:LYS:N	1.99	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:VAL:HG11	1:B:571:LEU:HD22	1.64	0.78
1:B:412:ILE:HD11	1:B:518:LEU:HD22	1.65	0.77
1:G:378:LYS:HG3	1:G:426:LEU:HD11	1.66	0.77
1:D:636:LEU:HD22	1:D:675:TYR:HB3	1.68	0.76
1:G:430:ASP:OD1	1:G:444:LYS:HG2	1.84	0.76
1:D:670:ILE:HD12	1:D:693:GLN:HB2	1.67	0.76
1:H:375:GLU:HG2	1:H:420:ARG:HB2	1.68	0.76
1:F:664:PRO:CG	1:F:687:ILE:HG12	2.15	0.75
1:I:411:GLY:HA3	1:I:564:ILE:HG13	1.66	0.75
1:B:549:LYS:HE2	1:B:584:THR:HG22	1.68	0.75
1:F:653:THR:HG23	1:F:654:ILE:CD1	2.13	0.75
1:G:411:GLY:HA3	1:G:564:ILE:HG13	1.68	0.75
1:F:612:VAL:HB	1:F:665:VAL:CG1	2.17	0.74
1:I:411:GLY:HA3	1:I:564:ILE:CG1	2.17	0.74
1:G:377:GLY:HA2	1:G:426:LEU:CG	2.17	0.74
1:I:362:ASN:N	1:I:363:PRO:HD2	2.02	0.74
1:C:655:THR:HG22	1:C:655:THR:O	1.86	0.74
1:F:657:THR:HB	1:F:662:GLN:HB2	1.70	0.74
1:E:372:VAL:HG21	1:E:417:ILE:HD13	1.70	0.73
1:I:549:LYS:HE3	1:I:584:THR:HG22	1.69	0.73
1:B:410:ILE:HG13	1:B:563:SER:HA	1.68	0.73
1:G:426:LEU:HD12	1:G:428:GLY:H	1.52	0.73
1:I:643:VAL:HG13	1:I:679:LEU:HD11	1.70	0.73
1:C:627:ILE:HG13	1:C:637:ALA:HB2	1.69	0.72
1:E:547:LEU:O	1:E:551:THR:HG23	1.90	0.72
1:I:543:ARG:HG2	1:I:543:ARG:O	1.90	0.71
1:C:664:PRO:HG2	1:C:687:ILE:HG12	1.72	0.71
1:E:452:THR:HG22	1:E:478:ALA:HB3	1.71	0.71
1:G:375:GLU:HG2	1:G:420:ARG:HB2	1.72	0.71
1:E:638:LEU:HB3	1:E:643:VAL:HG21	1.73	0.70
1:E:543:ARG:HG2	1:E:543:ARG:O	1.90	0.70
1:B:593:SER:HB2	1:B:693:GLN:HG2	1.73	0.70
1:F:664:PRO:HG3	1:F:687:ILE:HG12	1.71	0.70
1:E:636:LEU:CD2	1:E:638:LEU:HG	2.22	0.69
1:G:412:ILE:HD12	1:G:514:SER:CB	2.12	0.69
1:B:670:ILE:HD12	1:B:693:GLN:HB2	1.75	0.69
1:B:531:GLU:CG	1:B:538:VAL:HG11	2.22	0.69
1:F:494:LYS:HE3	1:F:495:TYR:H	1.56	0.69
1:F:612:VAL:CG1	1:F:665:VAL:CG1	2.65	0.68
1:F:612:VAL:CB	1:F:665:VAL:CG1	2.70	0.68
1:G:426:LEU:HD13	1:G:428:GLY:H	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:GLY:HA3	1:D:564:ILE:HG13	1.76	0.68
1:E:636:LEU:HD21	1:E:679:LEU:HD12	1.76	0.68
1:A:619:ILE:HD11	1:A:709:ILE:HG13	1.75	0.67
1:E:451:LEU:HD13	1:E:479:TRP:CE2	2.29	0.67
1:I:614:LEU:CD1	1:I:706:ARG:HE	2.08	0.67
1:I:526:MET:HE3	1:I:567:LEU:HD11	1.77	0.67
1:D:664:PRO:HG2	1:D:687:ILE:HG12	1.77	0.66
1:F:612:VAL:HB	1:F:665:VAL:HG12	1.78	0.66
1:E:664:PRO:HG2	1:E:687:ILE:HG12	1.77	0.66
1:D:411:GLY:HA3	1:D:564:ILE:CG1	2.25	0.66
1:A:619:ILE:O	1:A:623:ILE:HG13	1.96	0.66
1:D:628:LYS:HA	1:D:634:SER:HB3	1.77	0.65
1:I:614:LEU:HD12	1:I:706:ARG:HE	1.61	0.65
1:E:636:LEU:HD23	1:E:638:LEU:HG	1.79	0.65
1:H:378:LYS:H	1:H:426:LEU:HD22	1.61	0.65
1:C:543:ARG:O	1:C:543:ARG:HG2	1.95	0.64
1:G:410:ILE:HG23	1:G:412:ILE:H	1.61	0.64
1:B:381:SER:O	1:B:385:GLN:HG2	1.96	0.64
1:H:608:SER:HA	1:H:699:ILE:HD11	1.78	0.64
1:B:388:THR:HG22	1:B:389:LYS:H	1.61	0.64
1:A:549:LYS:HE2	1:A:584:THR:HG22	1.79	0.64
1:G:673:ARG:HG3	1:G:674:ARG:N	2.12	0.64
1:F:546:PRO:HD2	1:F:549:LYS:CD	2.13	0.63
1:H:402:MET:HE1	1:H:506:LEU:HB3	1.79	0.63
1:D:695:ILE:HD12	1:D:701:ILE:HD11	1.78	0.63
1:C:549:LYS:HE2	1:C:584:THR:HG22	1.80	0.63
1:C:670:ILE:HD12	1:C:693:GLN:HB2	1.81	0.63
1:G:412:ILE:HD11	1:G:558:VAL:CB	2.29	0.63
1:H:560:GLU:OE2	1:H:677:ARG:HG2	1.98	0.62
1:B:404:GLN:O	1:B:408:GLN:HG3	1.99	0.62
1:F:472:ALA:HB3	1:F:475:LEU:HG	1.81	0.62
1:A:627:ILE:HD12	1:A:635:TYR:HB2	1.82	0.62
1:H:549:LYS:HE2	1:H:584:THR:HG22	1.82	0.62
1:I:410:ILE:CG2	1:I:412:ILE:HD12	2.28	0.62
1:B:412:ILE:HD12	1:B:558:VAL:HG11	1.81	0.62
1:F:616:ASP:H	1:F:707:ILE:HG22	1.65	0.62
1:B:388:THR:CG2	1:B:389:LYS:N	2.63	0.61
1:H:642:SER:HA	1:H:645:LEU:HD12	1.81	0.61
1:E:464:LEU:HD12	1:E:465:PRO:CA	2.29	0.61
1:G:377:GLY:HA3	1:G:426:LEU:HD13	1.82	0.61
1:D:375:GLU:HG2	1:D:420:ARG:HB3	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:LEU:O	1:D:410:ILE:HG22	2.01	0.61
1:E:455:VAL:HG12	1:E:456:GLU:N	2.16	0.61
1:I:614:LEU:HB2	1:I:706:ARG:CG	2.30	0.61
1:A:388:THR:OG1	1:A:392:GLN:CG	2.45	0.60
1:A:388:THR:HG1	1:A:392:GLN:HG2	1.66	0.60
1:E:375:GLU:HG2	1:E:420:ARG:HB2	1.83	0.60
1:A:402:MET:HE3	1:A:507:SER:HA	1.83	0.59
1:A:623:ILE:O	1:A:623:ILE:HG22	2.02	0.59
1:B:388:THR:CG2	1:B:389:LYS:H	2.15	0.59
1:A:536:ASP:O	1:A:540[B]:GLU:HG2	2.03	0.59
1:I:664:PRO:HG2	1:I:687:ILE:HG12	1.85	0.59
1:F:612:VAL:CB	1:F:665:VAL:HG12	2.33	0.58
1:G:423:SER:HB3	1:G:426:LEU:HD23	1.83	0.58
1:G:583:ASP:OD1	1:G:585:VAL:HG12	2.03	0.58
1:C:673:ARG:HG3	1:C:674:ARG:N	2.17	0.58
1:D:619:ILE:O	1:D:623:ILE:HG12	2.03	0.58
1:E:541:VAL:HG11	1:E:571:LEU:HD22	1.85	0.58
1:F:585:VAL:O	1:F:589:GLU:HG2	2.03	0.58
1:E:465:PRO:HG3	1:E:481:SER:H	1.68	0.58
1:I:433:ILE:HB	1:I:441:VAL:HG12	1.85	0.58
1:F:465:PRO:HB2	1:F:481:SER:H	1.68	0.58
1:H:373:ILE:HB	1:H:434:LEU:HB2	1.84	0.58
1:A:402:MET:HE2	1:A:510:PHE:HD2	1.69	0.57
1:E:378:LYS:N	1:E:428:GLY:HA2	2.18	0.57
1:C:628:LYS:CG	1:C:634:SER:OG	2.46	0.57
1:F:411:GLY:H	1:F:564:ILE:H	1.51	0.57
1:C:626:ALA:HA	1:C:637:ALA:HB3	1.86	0.57
1:G:377:GLY:CA	1:G:426:LEU:HD13	2.34	0.57
1:B:455:VAL:HG12	1:B:456:GLU:N	2.20	0.57
1:G:412:ILE:CG1	1:G:558:VAL:HG11	2.35	0.57
1:C:410:ILE:HG23	1:C:412:ILE:H	1.69	0.57
1:G:423:SER:N	1:G:426:LEU:HD23	2.20	0.57
1:B:412:ILE:CD1	1:B:558:VAL:HG11	2.35	0.56
1:E:425:SER:O	1:E:426:LEU:HD12	2.06	0.56
1:F:635:TYR:OH	1:F:678:LYS:HE2	2.06	0.56
1:E:464:LEU:CD1	1:E:465:PRO:N	2.51	0.56
1:G:411:GLY:HA3	1:G:564:ILE:CG1	2.36	0.56
1:I:614:LEU:CD1	1:I:706:ARG:NH2	2.57	0.56
1:D:701:ILE:O	1:D:703:PRO:HD3	2.05	0.56
1:H:560:GLU:OE1	1:H:592:ARG:NH1	2.39	0.56
1:C:593:SER:O	1:C:596:LYS:HG3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:ILE:HD11	1:E:414:TYR:HE2	1.71	0.55
1:B:375:GLU:HG2	1:B:420:ARG:HB2	1.88	0.55
1:F:364:ASP:O	1:G:413:ARG:NH2	2.33	0.55
1:C:701:ILE:O	1:C:703:PRO:HD3	2.07	0.55
1:I:615:LEU:O	1:I:706:ARG:HD3	2.06	0.55
1:G:414:TYR:CD1	1:G:510:PHE:CD1	2.95	0.55
1:I:375:GLU:HG2	1:I:420:ARG:HB2	1.89	0.55
1:F:636:LEU:HD22	1:F:637:ALA:H	1.72	0.54
1:E:639:ASP:O	1:E:643:VAL:HG23	2.07	0.54
1:I:619:ILE:O	1:I:623:ILE:HG12	2.07	0.54
1:I:614:LEU:CB	1:I:706:ARG:HG2	2.35	0.54
1:C:462:TYR:HB3	1:C:464:LEU:HG	1.90	0.54
1:C:377:GLY:HA3	1:C:427:GLU:O	2.08	0.54
1:E:373:ILE:HB	1:E:434:LEU:HB2	1.90	0.54
1:B:620:GLU:O	1:B:624:ARG:HG3	2.07	0.53
1:F:448:HIS:O	1:F:482:GLU:HG2	2.08	0.53
1:F:515:GLN:HE22	1:F:558:VAL:HG23	1.73	0.53
1:H:673:ARG:HG3	1:H:674:ARG:N	2.23	0.53
1:F:543:ARG:HG2	1:F:543:ARG:O	2.07	0.53
1:A:402:MET:CE	1:A:510:PHE:HD2	2.20	0.53
1:I:362:ASN:N	1:I:363:PRO:HD3	2.21	0.53
1:D:593:SER:HB2	1:D:693:GLN:HG2	1.91	0.53
1:I:593:SER:HB2	1:I:693:GLN:HG2	1.91	0.53
1:I:365:ASP:OD1	1:I:365:ASP:C	2.47	0.53
1:E:455:VAL:HG12	1:E:457:ASP:H	1.74	0.53
1:F:531:GLU:HG3	1:F:538:VAL:HG11	1.90	0.53
1:A:413:ARG:HH21	1:I:365:ASP:HA	1.74	0.52
1:E:628:LYS:HD2	1:E:635:TYR:HB2	1.90	0.52
1:H:642:SER:HA	1:H:645:LEU:HB2	1.91	0.52
1:B:438:VAL:HG11	1:C:597:LEU:HG	1.90	0.52
1:F:662:GLN:N	1:F:663:PRO:HD3	2.24	0.52
1:H:444:LYS:HD2	1:H:469:TYR:OH	2.10	0.52
1:A:593:SER:HB2	1:A:693:GLN:HG2	1.92	0.52
1:A:627:ILE:HD11	1:A:637:ALA:HB2	1.91	0.52
1:I:647:LEU:HB3	1:I:651:ARG:NH1	2.24	0.52
1:F:616:ASP:HB3	1:F:619:ILE:HG12	1.92	0.52
1:G:664:PRO:HG2	1:G:687:ILE:HG12	1.90	0.52
1:E:411:GLY:CA	1:E:564:ILE:HG12	2.33	0.52
1:F:658:PRO:HG2	1:F:662:GLN:HG3	1.90	0.52
1:B:459:LEU:HD21	1:B:466:PHE:HB3	1.92	0.51
1:B:597:LEU:HD12	1:B:696:LEU:HD11	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:592:ARG:NE	1:D:694:GLU:OE1	2.42	0.51
1:F:612:VAL:HA	1:F:665:VAL:HG12	1.92	0.51
1:H:378:LYS:N	1:H:426:LEU:HD22	2.24	0.51
1:G:379:ASP:HB3	1:G:429:TYR:CZ	2.45	0.51
1:B:576:GLU:HB2	2:B:801:GOL:H2	1.93	0.51
1:E:587:LEU:O	1:E:591:VAL:HG23	2.10	0.51
1:I:388:THR:HG22	3:I:905:HOH:O	2.10	0.51
1:E:628:LYS:HB2	1:E:635:TYR:H	1.75	0.51
1:H:531:GLU:HG3	1:H:538:VAL:HG11	1.92	0.51
1:C:628:LYS:HG3	1:C:634:SER:HG	1.68	0.51
1:G:592:ARG:NE	1:G:673:ARG:HH21	2.09	0.51
1:G:426:LEU:HD12	1:G:426:LEU:C	2.32	0.51
1:E:372:VAL:CG2	1:E:417:ILE:HD13	2.40	0.50
1:G:372:VAL:HG21	1:G:417:ILE:HD13	1.94	0.50
1:C:537:LEU:O	1:C:541:VAL:HG23	2.12	0.50
1:A:619:ILE:HD12	1:A:646:ILE:HG12	1.94	0.50
1:I:411:GLY:HA3	1:I:564:ILE:HG12	1.90	0.50
1:B:648:LYS:HG3	1:B:651:ARG:HH21	1.76	0.50
1:B:658:PRO:HG2	1:B:661:GLY:HA3	1.93	0.50
1:F:465:PRO:CB	1:F:481:SER:H	2.24	0.50
1:I:583:ASP:OD1	1:I:585:VAL:HG12	2.12	0.50
1:C:541:VAL:HG21	1:C:571:LEU:HB3	1.94	0.49
1:F:619:ILE:HG13	1:F:707:ILE:CG2	2.42	0.49
1:H:426:LEU:HD13	1:H:428:GLY:N	2.27	0.49
1:E:602:LYS:HD3	1:E:603:PHE:CZ	2.47	0.49
1:F:426:LEU:HD11	1:F:432:MET:HB2	1.95	0.49
1:H:432:MET:HE2	1:H:434:LEU:HD11	1.94	0.49
1:E:452:THR:HG23	1:E:454:GLU:H	1.78	0.49
1:D:593:SER:O	1:D:596:LYS:HG3	2.12	0.49
1:H:466:PHE:HA	1:H:479:TRP:O	2.13	0.49
1:E:372:VAL:HG23	1:E:417:ILE:HA	1.94	0.49
1:F:672:VAL:O	1:F:676:VAL:HG23	2.12	0.49
1:E:455:VAL:CG1	1:E:456:GLU:N	2.76	0.49
1:E:528:GLU:HG3	1:E:529:PHE:N	2.27	0.49
1:G:377:GLY:HA2	1:G:426:LEU:HD22	0.61	0.49
1:H:614:LEU:CD2	1:H:667:LEU:HB3	2.42	0.49
1:F:657:THR:CG2	1:F:662:GLN:O	2.58	0.49
1:H:410:ILE:HG23	1:H:412:ILE:H	1.77	0.49
1:A:396:ASP:O	1:A:400:PRO:HG2	2.13	0.48
1:G:380:LEU:HG	1:G:429:TYR:HA	1.94	0.48
1:H:375:GLU:HG2	1:H:420:ARG:CB	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ASP:O	1:C:413:ARG:HD2	2.13	0.48
1:B:541:VAL:CG2	1:B:575:SER:HB2	2.43	0.48
1:E:636:LEU:O	1:E:638:LEU:HD12	2.13	0.48
1:H:445:ILE:HG21	1:H:498:PRO:HB3	1.96	0.48
1:G:412:ILE:HG12	1:G:558:VAL:HG11	1.94	0.48
1:B:541:VAL:HG11	1:B:571:LEU:CD2	2.40	0.48
1:C:674:ARG:O	1:C:677:ARG:HB3	2.13	0.48
1:E:523:VAL:HG11	1:E:551:THR:HG22	1.96	0.48
1:B:455:VAL:CG1	1:B:456:GLU:N	2.77	0.48
1:F:657:THR:HB	1:F:662:GLN:CB	2.40	0.48
1:E:636:LEU:HG	1:E:638:LEU:HG	1.96	0.47
1:F:524:ARG:HB2	1:F:547:LEU:HD21	1.95	0.47
1:E:576:GLU:HB2	2:E:801:GOL:H32	1.95	0.47
1:F:429:TYR:CZ	1:F:447:PRO:HB3	2.49	0.47
1:G:394:PHE:HB2	1:G:499:LEU:HD13	1.96	0.47
1:C:474:GLY:O	1:C:475:LEU:HD23	2.14	0.47
1:D:410:ILE:HD11	1:D:558:VAL:HB	1.95	0.47
1:G:540:GLU:HA	1:G:540:GLU:OE1	2.14	0.47
1:H:402:MET:HE2	1:H:510:PHE:HD2	1.79	0.47
1:B:628:LYS:HD2	1:B:635:TYR:CE2	2.49	0.47
1:G:455:VAL:HG12	1:G:456:GLU:N	2.30	0.47
1:F:523:VAL:HA	1:F:526:MET:CE	2.44	0.47
1:I:451:LEU:HD13	1:I:479:TRP:CE2	2.50	0.47
1:D:410:ILE:HG21	1:D:414:TYR:OH	2.15	0.47
1:D:411:GLY:HA3	1:D:564:ILE:HG12	1.96	0.47
1:G:593:SER:HB2	1:G:693:GLN:HG2	1.97	0.47
1:H:596:LYS:HE3	1:H:693:GLN:O	2.15	0.47
1:A:445:ILE:HG21	1:A:498:PRO:HB3	1.96	0.47
1:A:579:GLN:NE2	1:I:548:GLN:HG3	2.30	0.47
1:A:664:PRO:HG2	1:A:687:ILE:HG12	1.96	0.47
1:D:435:LEU:HD21	1:D:516:GLU:HG3	1.97	0.47
1:G:378:LYS:CG	1:G:426:LEU:HD11	2.41	0.47
1:B:388:THR:HG22	1:B:392:GLN:HB3	1.96	0.47
1:C:597:LEU:HD12	1:C:696:LEU:HD11	1.97	0.47
1:A:377:GLY:HA3	1:A:427:GLU:O	2.15	0.47
1:C:452:THR:O	1:C:478:ALA:HB3	2.14	0.47
1:C:651:ARG:O	1:C:654:ILE:HG13	2.15	0.47
1:E:373:ILE:HD13	1:E:418:HIS:HB2	1.97	0.47
1:F:630:THR:HG22	1:F:634:SER:HA	1.96	0.47
1:H:524:ARG:HB2	1:H:547:LEU:HD21	1.97	0.47
1:I:488:LEU:HD22	1:I:493:ILE:HG21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:LEU:HD13	1:F:502:ILE:HD11	1.97	0.47
1:H:380:LEU:HD12	1:H:430:ASP:O	2.16	0.47
1:C:593:SER:HB2	1:C:693:GLN:HG2	1.97	0.46
1:E:593:SER:HB2	1:E:693:GLN:HG2	1.97	0.46
1:F:373:ILE:HG12	1:F:418:HIS:HB2	1.96	0.46
1:G:399:ILE:HB	1:G:400:PRO:HD3	1.97	0.46
1:G:673:ARG:NH1	1:G:674:ARG:HA	2.31	0.46
1:H:402:MET:HE3	1:H:507:SER:HA	1.97	0.46
1:H:672:VAL:HA	1:H:675:TYR:HD2	1.81	0.46
1:B:432:MET:HE3	1:B:434:LEU:HD11	1.97	0.46
1:H:388:THR:HG23	1:H:391:GLY:HA3	1.98	0.46
1:A:643:VAL:HG22	1:A:679:LEU:HD11	1.98	0.46
1:D:653:THR:HG21	1:D:706:ARG:O	2.16	0.46
1:G:592:ARG:CD	1:G:673:ARG:HH21	2.29	0.46
1:A:596:LYS:HE3	1:A:693:GLN:O	2.16	0.46
1:E:458:ASN:O	1:E:461:ARG:HG3	2.16	0.46
1:H:431:TYR:CZ	1:H:443:GLY:HA3	2.51	0.46
1:A:407:TYR:CE2	1:A:565:LYS:HE2	2.51	0.46
1:G:423:SER:CA	1:G:426:LEU:HD23	2.46	0.46
1:H:589:GLU:HA	1:H:589:GLU:OE1	2.15	0.46
1:I:614:LEU:HD13	1:I:706:ARG:CZ	2.46	0.46
1:H:378:LYS:HG3	1:H:426:LEU:HD21	1.98	0.45
1:H:454:GLU:HG2	1:H:493:ILE:HG23	1.98	0.45
1:H:526:MET:HB2	1:H:526:MET:HE2	1.53	0.45
1:I:648:LYS:HG2	1:I:651:ARG:NH2	2.31	0.45
1:E:465:PRO:HB2	1:E:480:VAL:HA	1.98	0.45
1:F:411:GLY:CA	1:F:564:ILE:HG12	2.24	0.45
1:G:377:GLY:CA	1:G:426:LEU:CD2	2.42	0.45
1:A:623:ILE:HD11	1:A:646:ILE:HD13	1.98	0.45
1:E:531:GLU:HG3	1:E:538:VAL:HG11	1.98	0.45
1:F:515:GLN:NE2	1:F:558:VAL:HG23	2.31	0.45
1:I:670:ILE:CD1	1:I:693:GLN:HB2	2.47	0.45
1:D:410:ILE:HG12	1:D:412:ILE:HD12	1.99	0.45
1:H:411:GLY:HA3	1:H:564:ILE:HG13	1.98	0.45
1:A:383:LEU:HD12	1:A:383:LEU:HA	1.77	0.45
1:A:614:LEU:HD12	1:A:706:ARG:HE	1.81	0.45
1:G:523:VAL:HG21	1:G:551:THR:HG23	1.99	0.45
1:I:593:SER:O	1:I:596:LYS:HG3	2.16	0.45
1:D:628:LYS:HB3	1:D:628:LYS:HE3	1.78	0.45
1:E:452:THR:HB	1:E:478:ALA:O	2.17	0.45
1:F:635:TYR:OH	1:F:678:LYS:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:423:SER:O	1:H:426:LEU:HD23	2.16	0.45
1:B:684:PHE:HB3	1:B:687:ILE:HD12	1.99	0.45
1:F:518:LEU:HD23	1:F:555:LYS:HG2	1.98	0.45
1:H:526:MET:HE1	1:H:554:PHE:HD2	1.82	0.45
1:A:457:ASP:O	1:A:461:ARG:HG3	2.16	0.45
1:E:520:ILE:HA	1:E:551:THR:HG21	1.99	0.45
1:F:589:GLU:OE1	1:F:674:ARG:HB3	2.16	0.45
1:F:681:GLU:HA	1:F:685:PRO:HA	1.99	0.45
1:G:373:ILE:HD13	1:G:418:HIS:HB2	1.97	0.45
1:E:464:LEU:C	1:E:464:LEU:HD12	2.34	0.45
1:F:365:ASP:HA	1:G:413:ARG:NH2	2.32	0.45
1:G:531:GLU:HG3	1:G:538:VAL:HG11	1.98	0.45
1:I:468:THR:HA	1:I:477:SER:O	2.17	0.45
1:C:655:THR:CG2	1:C:655:THR:O	2.58	0.44
1:I:456:GLU:HB3	1:I:466:PHE:CZ	2.52	0.44
1:C:445:ILE:HD13	1:C:498:PRO:HB3	1.98	0.44
1:H:380:LEU:HD23	1:H:383:LEU:HD12	1.99	0.44
1:A:627:ILE:HG22	1:A:629:GLN:HG3	1.98	0.44
1:B:497:THR:O	1:B:501:VAL:HG23	2.17	0.44
1:C:375:GLU:HG2	1:C:420:ARG:HB2	1.98	0.44
1:G:497:THR:OG1	1:G:500:GLU:HG3	2.17	0.44
1:H:530:MET:HG2	1:H:567:LEU:HD13	2.00	0.44
1:I:445:ILE:HG21	1:I:498:PRO:HB3	2.00	0.44
1:E:470:LYS:HG2	1:E:472:ALA:O	2.17	0.44
1:F:638:LEU:HA	1:F:638:LEU:HD23	1.86	0.44
1:E:567:LEU:HD23	1:E:567:LEU:HA	1.84	0.44
1:G:410:ILE:HG23	1:G:412:ILE:N	2.29	0.44
1:H:665:VAL:HG13	1:H:690:ILE:HD13	1.99	0.44
1:A:529:PHE:CE1	1:I:366:TYR:O	2.71	0.44
1:C:396:ASP:O	1:C:400:PRO:HG2	2.17	0.44
1:I:515:GLN:NE2	1:I:559:GLN:HB2	2.32	0.44
1:B:530:MET:HG2	1:B:567:LEU:HD13	2.00	0.44
1:H:494:LYS:HD2	1:H:496:TRP:CZ2	2.52	0.44
1:A:628:LYS:HB2	1:A:628:LYS:HE3	1.76	0.44
1:B:616:ASP:OD2	1:B:708:GLN:HG3	2.18	0.44
1:E:557:LEU:HD11	1:E:591:VAL:HG11	1.99	0.44
1:G:423:SER:CB	1:G:426:LEU:HD23	2.47	0.44
1:I:614:LEU:CD1	1:I:706:ARG:NE	2.78	0.44
1:C:615:LEU:HD23	1:C:707:ILE:HB	2.00	0.44
1:F:465:PRO:HB2	1:F:481:SER:N	2.32	0.44
1:I:429:TYR:CE2	1:I:447:PRO:HB3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:673:ARG:HG3	1:F:674:ARG:N	2.33	0.43
1:A:399:ILE:HB	1:A:400:PRO:HD3	2.00	0.43
1:A:402:MET:HE2	1:A:510:PHE:CD2	2.52	0.43
1:C:423:SER:HB3	1:C:426:LEU:HB2	2.00	0.43
1:E:379:ASP:HB2	1:E:428:GLY:O	2.18	0.43
1:E:636:LEU:HD23	1:E:638:LEU:CG	2.48	0.43
1:G:616:ASP:HB2	1:G:707:ILE:O	2.19	0.43
1:H:368:LEU:HD12	1:H:368:LEU:HA	1.83	0.43
1:D:616:ASP:HB2	1:D:707:ILE:O	2.18	0.43
1:F:446:PRO:HA	1:F:447:PRO:HD3	1.79	0.43
1:C:639:ASP:O	1:C:643:VAL:HG23	2.17	0.43
1:G:557:LEU:HD11	1:G:591:VAL:HG11	2.00	0.43
1:A:446:PRO:HA	1:A:447:PRO:HD3	1.92	0.43
1:E:520:ILE:HD11	1:E:548:GLN:HG2	2.01	0.43
1:B:388:THR:CG2	1:B:392:GLN:HB3	2.48	0.43
1:B:429:TYR:CD2	1:B:447:PRO:HG3	2.53	0.43
1:B:670:ILE:CD1	1:B:693:GLN:HB2	2.47	0.43
1:F:589:GLU:CD	1:F:674:ARG:HB3	2.39	0.43
1:B:664:PRO:HG2	1:B:687:ILE:HG12	2.01	0.43
1:G:430:ASP:CG	1:G:444:LYS:HG2	2.39	0.43
1:I:484:ALA:O	1:I:488:LEU:HG	2.19	0.43
1:I:648:LYS:HA	1:I:651:ARG:NH2	2.34	0.43
1:B:582:LYS:HA	1:B:582:LYS:HD3	1.77	0.43
1:A:402:MET:HE3	1:A:507:SER:CA	2.47	0.43
1:D:445:ILE:HG21	1:D:498:PRO:HB3	2.00	0.43
1:G:423:SER:H	1:G:426:LEU:HD23	1.84	0.43
1:B:636:LEU:HD21	1:B:679:LEU:HD12	2.01	0.42
1:E:636:LEU:CG	1:E:638:LEU:HG	2.50	0.42
1:F:587:LEU:O	1:F:591:VAL:HG23	2.19	0.42
1:I:526:MET:CE	1:I:567:LEU:HD21	2.50	0.42
1:E:423:SER:OG	1:E:426:LEU:HD13	2.20	0.42
1:E:472:ALA:HB3	1:E:475:LEU:HG	2.01	0.42
1:E:523:VAL:HA	1:E:526:MET:HG2	2.01	0.42
1:F:375:GLU:HG2	1:F:420:ARG:HB2	2.00	0.42
1:F:570:ILE:HG23	1:F:591:VAL:HG11	2.02	0.42
1:F:612:VAL:CA	1:F:665:VAL:HG12	2.49	0.42
1:G:451:LEU:HD13	1:G:479:TRP:CE2	2.55	0.42
1:D:399:ILE:HB	1:D:400:PRO:HD3	2.02	0.42
1:G:414:TYR:CE1	1:G:510:PHE:HB3	2.55	0.42
1:C:459:LEU:HD21	1:C:478:ALA:HB1	2.02	0.42
1:C:497:THR:O	1:C:501:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:THR:CG2	1:E:454:GLU:H	2.32	0.42
1:E:515:GLN:NE2	1:E:559:GLN:HB2	2.35	0.42
1:F:610:ILE:HG12	1:F:612:VAL:HG13	2.02	0.42
1:F:624:ARG:O	1:F:637:ALA:HB3	2.19	0.42
1:B:407:TYR:CG	1:B:407:TYR:O	2.73	0.42
1:C:411:GLY:HA3	1:C:564:ILE:HG13	2.02	0.42
1:D:377:GLY:HA3	1:D:427:GLU:O	2.20	0.42
1:F:398:MET:HB3	1:F:503:ILE:HG13	2.01	0.42
1:B:639:ASP:O	1:B:643:VAL:HG23	2.20	0.42
1:G:445:ILE:HD13	1:G:498:PRO:HB3	2.01	0.42
1:B:411:GLY:O	1:B:564:ILE:HG13	2.20	0.42
1:C:462:TYR:CZ	1:C:487:ILE:HG12	2.55	0.42
1:H:451:LEU:HD13	1:H:479:TRP:CE2	2.55	0.42
1:I:373:ILE:HB	1:I:434:LEU:HB2	2.02	0.42
1:A:397:ASP:O	1:A:401:LYS:HG2	2.20	0.41
1:C:614:LEU:HD23	1:C:667:LEU:HB3	2.01	0.41
1:F:381:SER:HB3	1:F:421:THR:HB	2.01	0.41
1:G:568:ARG:O	1:G:572:GLU:HB2	2.20	0.41
1:H:690:ILE:HG22	1:H:691:SER:N	2.35	0.41
2:A:802:GOL:C3	1:I:548:GLN:HE21	2.32	0.41
1:H:615:LEU:HG	1:H:666:LEU:HD11	2.02	0.41
1:B:445:ILE:HG21	1:B:498:PRO:HB3	2.02	0.41
1:C:432:MET:HB3	1:C:432:MET:HE2	1.83	0.41
1:D:557:LEU:HD11	1:D:591:VAL:HG11	2.03	0.41
1:E:419:VAL:O	1:E:419:VAL:HG13	2.20	0.41
1:E:455:VAL:CG1	1:E:456:GLU:H	2.33	0.41
1:B:542:THR:O	1:B:542:THR:HG22	2.20	0.41
1:C:589:GLU:HA	1:C:589:GLU:OE1	2.19	0.41
1:D:639:ASP:O	1:D:643:VAL:HG23	2.21	0.41
1:E:408:GLN:OE1	1:E:565:LYS:HE3	2.20	0.41
1:E:684:PHE:HB3	1:E:687:ILE:HD12	2.02	0.41
1:F:529:PHE:HD1	1:F:532:ARG:HH21	1.68	0.41
1:B:455:VAL:CG1	1:B:456:GLU:H	2.33	0.41
1:I:603:PHE:HB3	1:I:665:VAL:HG21	2.02	0.41
1:A:426:LEU:HD22	1:A:430:ASP:HB3	2.02	0.41
1:B:645:LEU:HD23	1:B:709:ILE:HG21	2.03	0.41
1:B:619:ILE:HD12	1:B:646:ILE:HG12	2.01	0.41
1:C:528:GLU:O	1:C:531:GLU:HB2	2.21	0.41
1:D:453:ASN:HB3	1:D:494:LYS:HE3	2.01	0.41
1:D:643:VAL:O	1:D:647:LEU:HD13	2.20	0.41
1:A:383:LEU:O	1:A:499:LEU:HD11	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:LYS:HB2	1:B:469:TYR:OH	2.21	0.41
1:D:592:ARG:HB3	1:D:694:GLU:OE1	2.21	0.41
1:F:523:VAL:HA	1:F:526:MET:HE2	2.02	0.41
1:C:567:LEU:HA	1:C:567:LEU:HD23	1.77	0.41
1:C:670:ILE:CD1	1:C:693:GLN:HB2	2.49	0.41
1:F:380:LEU:HD23	1:F:380:LEU:HA	1.88	0.41
1:F:534:PHE:HB3	1:F:537:LEU:HB3	2.03	0.41
1:H:552:GLU:O	1:H:556:ARG:HG3	2.21	0.41
1:H:618:GLU:O	1:H:622:MET:HB2	2.20	0.41
1:F:619:ILE:HG13	1:F:707:ILE:HG23	2.03	0.41
1:H:548:GLN:HG2	1:I:579:GLN:NE2	2.36	0.41
1:C:438:VAL:HG11	1:D:597:LEU:HG	2.03	0.41
1:E:676:VAL:O	1:E:680:ILE:HG23	2.21	0.41
1:A:602:LYS:HD3	1:A:603:PHE:CZ	2.55	0.41
1:D:383:LEU:HD12	1:D:383:LEU:HA	1.78	0.41
1:E:412:ILE:H	1:E:412:ILE:HD12	1.86	0.41
1:D:446:PRO:HA	1:D:447:PRO:HD3	1.92	0.40
1:G:426:LEU:HD13	1:G:428:GLY:N	2.31	0.40
1:I:531:GLU:HG3	1:I:538:VAL:HG11	2.03	0.40
1:D:696:LEU:O	1:D:699:ILE:HG22	2.22	0.40
1:E:459:LEU:HD23	1:E:459:LEU:HA	1.79	0.40
1:B:411:GLY:HA3	1:B:564:ILE:HG13	2.04	0.40
1:C:602:LYS:HD3	1:C:603:PHE:CE1	2.57	0.40
1:C:619:ILE:O	1:C:623:ILE:HG12	2.21	0.40
1:F:399:ILE:HB	1:F:400:PRO:HD3	2.03	0.40
1:F:593:SER:HB2	1:F:693:GLN:HG2	2.04	0.40
1:H:593:SER:HB2	1:H:693:GLN:HG2	2.02	0.40
1:I:446:PRO:HA	1:I:447:PRO:HD3	1.91	0.40
1:B:602:LYS:HD3	1:B:603:PHE:CZ	2.56	0.40
1:B:651:ARG:NH1	1:B:683:GLU:OE2	2.54	0.40
1:A:650:MET:HG3	1:A:707:ILE:HD12	2.04	0.40
1:B:605:GLN:NE2	1:B:662:GLN:HB2	2.36	0.40
1:C:417:ILE:HD11	1:C:510:PHE:HE2	1.86	0.40
1:E:427:GLU:HG3	1:E:430:ASP:OD2	2.21	0.40
1:F:655:THR:HA	1:F:656:PRO:HD3	1.95	0.40
1:G:446:PRO:HA	1:G:447:PRO:HD3	1.95	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	351/387 (91%)	344 (98%)	7 (2%)	0	100	100
1	B	345/387 (89%)	331 (96%)	14 (4%)	0	100	100
1	C	336/387 (87%)	321 (96%)	15 (4%)	0	100	100
1	D	341/387 (88%)	329 (96%)	12 (4%)	0	100	100
1	E	339/387 (88%)	323 (95%)	16 (5%)	0	100	100
1	F	337/387 (87%)	313 (93%)	24 (7%)	0	100	100
1	G	340/387 (88%)	329 (97%)	11 (3%)	0	100	100
1	H	314/387 (81%)	300 (96%)	14 (4%)	0	100	100
1	I	331/387 (86%)	320 (97%)	11 (3%)	0	100	100
All	All	3034/3483 (87%)	2910 (96%)	124 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	323/345 (94%)	310 (96%)	13 (4%)	31	65
1	B	317/345 (92%)	305 (96%)	12 (4%)	33	67
1	C	314/345 (91%)	308 (98%)	6 (2%)	57	85
1	D	318/345 (92%)	315 (99%)	3 (1%)	78	94
1	E	316/345 (92%)	305 (96%)	11 (4%)	36	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	313/345 (91%)	304 (97%)	9 (3%)	42	76
1	G	314/345 (91%)	306 (98%)	8 (2%)	47	80
1	H	299/345 (87%)	291 (97%)	8 (3%)	44	78
1	I	313/345 (91%)	305 (97%)	8 (3%)	46	79
All	All	2827/3105 (91%)	2749 (97%)	78 (3%)	44	77

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402	MET
1	A	463	ASN
1	A	494	LYS
1	A	497	THR
1	A	503	ILE
1	A	524	ARG
1	A	530	MET
1	A	540[A]	GLU
1	A	540[B]	GLU
1	A	543	ARG
1	A	634	SER
1	A	639	ASP
1	A	700	ARG
1	B	409	ASP
1	B	410	ILE
1	B	412	ILE
1	B	413	ARG
1	B	442	ARG
1	B	524	ARG
1	B	528	GLU
1	B	530	MET
1	B	585	VAL
1	B	618	GLU
1	B	627	ILE
1	B	634	SER
1	C	365	ASP
1	C	426	LEU
1	C	460	SER
1	C	530	MET
1	C	594	SER
1	C	621	GLU
1	D	367	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	530	MET
1	D	594	SER
1	E	365	ASP
1	E	426	LEU
1	E	452	THR
1	E	511	HIS
1	E	528	GLU
1	E	530	MET
1	E	540	GLU
1	E	543	ARG
1	E	655	THR
1	E	657	THR
1	E	673	ARG
1	F	461	ARG
1	F	494	LYS
1	F	543	ARG
1	F	548	GLN
1	F	565	LYS
1	F	636	LEU
1	F	638	LEU
1	F	673	ARG
1	F	700	ARG
1	G	365	ASP
1	G	372	VAL
1	G	383	LEU
1	G	410	ILE
1	G	524	ARG
1	G	542	THR
1	G	662	GLN
1	G	673	ARG
1	H	364	ASP
1	H	388	THR
1	H	392	GLN
1	H	421	THR
1	H	422	ASP
1	H	455	VAL
1	H	575	SER
1	H	585	VAL
1	I	389	LYS
1	I	395	VAL
1	I	524	ARG
1	I	530	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	543	ARG
1	I	649	SER
1	I	680	ILE
1	I	708	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

13 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	GOL	C	801	-	5,5,5	0.09	0	5,5,5	0.32	0
2	GOL	A	801	-	5,5,5	0.10	0	5,5,5	0.32	0
2	GOL	G	801	-	5,5,5	0.09	0	5,5,5	0.32	0
2	GOL	A	802	-	5,5,5	0.09	0	5,5,5	0.32	0
2	GOL	E	801	-	5,5,5	0.08	0	5,5,5	0.32	0
2	GOL	E	802	-	5,5,5	0.08	0	5,5,5	0.32	0
2	GOL	B	802	-	5,5,5	0.09	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	B	801	-	5,5,5	0.09	0	5,5,5	0.32	0
2	GOL	A	803	-	5,5,5	0.08	0	5,5,5	0.32	0
2	GOL	D	801	-	5,5,5	0.10	0	5,5,5	0.32	0
2	GOL	E	803	-	5,5,5	0.09	0	5,5,5	0.32	0
2	GOL	I	801	-	5,5,5	0.09	0	5,5,5	0.32	0
2	GOL	A	804	-	5,5,5	0.09	0	5,5,5	0.32	0

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
2	GOL	C	801	-	-	0/4/4/4	-
2	GOL	A	801	-	-	2/4/4/4	-
2	GOL	G	801	-	-	2/4/4/4	-
2	GOL	A	802	-	-	2/4/4/4	-
2	GOL	E	801	-	-	1/4/4/4	-
2	GOL	E	802	-	-	4/4/4/4	-
2	GOL	B	802	-	-	2/4/4/4	-
2	GOL	B	801	-	-	2/4/4/4	-
2	GOL	A	803	-	-	3/4/4/4	-
2	GOL	D	801	-	-	2/4/4/4	-
2	GOL	E	803	-	-	2/4/4/4	-
2	GOL	I	801	-	-	2/4/4/4	-
2	GOL	A	804	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	802	GOL	O1-C1-C2-C3
2	E	802	GOL	O1-C1-C2-C3
2	E	802	GOL	C1-C2-C3-O3
2	A	803	GOL	O1-C1-C2-O2
2	I	801	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	801	GOL	O2-C2-C3-O3
2	A	801	GOL	C1-C2-C3-O3
2	G	801	GOL	C1-C2-C3-O3
2	B	802	GOL	O1-C1-C2-C3
2	B	801	GOL	O1-C1-C2-C3
2	A	803	GOL	O1-C1-C2-C3
2	D	801	GOL	C1-C2-C3-O3
2	E	803	GOL	O1-C1-C2-C3
2	A	804	GOL	O1-C1-C2-C3
2	E	802	GOL	O2-C2-C3-O3
2	E	803	GOL	O1-C1-C2-O2
2	A	804	GOL	O1-C1-C2-O2
2	A	802	GOL	O1-C1-C2-O2
2	E	802	GOL	O1-C1-C2-O2
2	A	801	GOL	O2-C2-C3-O3
2	E	801	GOL	O2-C2-C3-O3
2	A	803	GOL	O2-C2-C3-O3
2	A	804	GOL	O2-C2-C3-O3
2	D	801	GOL	O2-C2-C3-O3
2	I	801	GOL	O2-C2-C3-O3
2	B	801	GOL	O1-C1-C2-O2
2	B	802	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	GOL	1	0
2	E	801	GOL	1	0
2	B	801	GOL	1	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	348/387 (89%)	-0.13	2 (0%)	89	86	37, 61, 109, 201	0
1	B	347/387 (89%)	-0.01	6 (1%)	70	63	36, 77, 154, 225	0
1	C	342/387 (88%)	0.06	7 (2%)	65	56	48, 104, 185, 241	0
1	D	343/387 (88%)	-0.06	5 (1%)	73	68	42, 75, 149, 224	0
1	E	343/387 (88%)	-0.08	8 (2%)	60	51	44, 92, 166, 238	0
1	F	340/387 (87%)	0.01	9 (2%)	56	46	30, 106, 182, 239	0
1	G	343/387 (88%)	0.03	6 (1%)	70	63	58, 89, 148, 233	0
1	H	320/387 (82%)	0.20	14 (4%)	34	24	62, 117, 189, 247	0
1	I	334/387 (86%)	-0.05	11 (3%)	46	36	48, 95, 171, 211	0
All	All	3060/3483 (87%)	-0.01	68 (2%)	62	52	30, 89, 171, 247	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	632	ALA	7.5
1	F	632	ALA	6.6
1	F	635	TYR	4.8
1	F	464	LEU	4.4
1	H	648	LYS	4.3
1	B	632	ALA	4.2
1	C	632	ALA	4.1
1	F	660	GLY	4.0
1	F	659	ALA	3.8
1	D	627	ILE	3.8
1	A	630	THR	3.8
1	H	650	MET	3.7
1	E	630	THR	3.6
1	B	408	GLN	3.4
1	H	463	ASN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	468	THR	3.2
1	C	633	GLY	3.2
1	A	628	LYS	3.1
1	B	411	GLY	3.1
1	B	634	SER	3.0
1	C	646	ILE	2.9
1	H	462	TYR	2.9
1	H	646	ILE	2.9
1	G	659	ALA	2.9
1	E	386	HIS	2.9
1	H	610	ILE	2.9
1	F	650	MET	2.9
1	I	646	ILE	2.8
1	B	542	THR	2.8
1	C	462	TYR	2.8
1	E	635	TYR	2.7
1	G	650	MET	2.7
1	F	640	PRO	2.7
1	I	610	ILE	2.6
1	I	362	ASN	2.6
1	G	661	GLY	2.6
1	E	629	GLN	2.5
1	E	462	TYR	2.5
1	I	410	ILE	2.5
1	I	614	LEU	2.5
1	H	700	ARG	2.4
1	E	466	PHE	2.4
1	H	445	ILE	2.4
1	I	411	GLY	2.4
1	H	609	ALA	2.4
1	B	635	TYR	2.4
1	D	629	GLN	2.4
1	I	363	PRO	2.3
1	I	706	ARG	2.3
1	I	645	LEU	2.3
1	H	678	LYS	2.3
1	H	603	PHE	2.3
1	G	652	ASN	2.2
1	F	664	PRO	2.2
1	D	633	GLY	2.2
1	I	679	LEU	2.2
1	H	485	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	635	TYR	2.2
1	H	509	PHE	2.2
1	H	440	TYR	2.2
1	G	619	ILE	2.1
1	F	641	ASP	2.1
1	I	650	MET	2.1
1	G	648	LYS	2.1
1	D	411	GLY	2.0
1	E	465	PRO	2.0
1	E	417	ILE	2.0
1	C	636	LEU	2.0

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
2	GOL	C	801	6/6	0.59	0.26	155,158,162,165	0
2	GOL	G	801	6/6	0.68	0.36	110,114,116,117	0
2	GOL	B	802	6/6	0.75	0.41	99,109,112,113	0
2	GOL	I	801	6/6	0.80	0.20	105,120,127,131	0
2	GOL	A	804	6/6	0.81	0.34	66,79,82,82	0
2	GOL	E	801	6/6	0.82	0.33	79,94,112,117	0
2	GOL	E	803	6/6	0.83	0.32	117,121,136,139	0
2	GOL	E	802	6/6	0.84	0.38	65,75,84,90	0
2	GOL	D	801	6/6	0.85	0.21	75,98,101,102	0
2	GOL	A	802	6/6	0.88	0.46	75,101,102,105	0
2	GOL	A	801	6/6	0.90	0.17	85,96,112,118	0
2	GOL	A	803	6/6	0.90	0.12	87,98,105,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	B	801	6/6	0.91	0.25	68,75,85,90	0

6.5 Other polymers (i)

There are no such residues in this entry.