Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:38 PM EDT

PDB ID	:	1KNO
Title	:	CRYSTAL STRUCTURE OF THE COMPLEX OF A CATALYTIC ANTIBODY FAB WITH A TRANSITION STATE ANALOG: STRUCTURAL SIMILARITIES IN ESTERASE-LIKE ABZYMES
Authors	:	Charbonnier, J.-B.; Gigant, B.; Knossow, M.
Deposited on	:	1995-09-11
Resolution	:	3.20 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 (i)) were used in the production of this report:

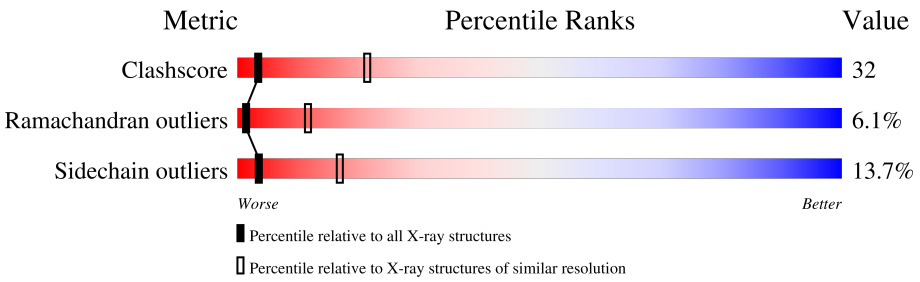
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.20 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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	47% 44% 8%
1	C	214	45% 45% 10%
1	E	214	50% 43% 8%
2	B	220	38% 52% 9% •
2	D	220	38% 52% 9% •
2	F	220	41% 50% 8% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9949 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 IGG2A FAB FRAGMENT CNJ206.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1655	1026	277	345	7	0	0	0
			Total	C	N	O	S			
1	C	214	1655	1026	277	345	7	0	0	0
			Total	C	N	O	S			
1	E	214	1655	1026	277	345	7	0	0	0

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLU	ASP	CONFLICT	GB 12002892
A	30	SER	GLY	CONFLICT	GB 12002892
A	31	GLY	VAL	CONFLICT	GB 12002892
A	32	TYR	SER	CONFLICT	GB 12002892
A	34	SER	ASN	CONFLICT	GB 12002892
A	39	LYS	GLU	CONFLICT	GB 12002892
A	50	ALA	GLY	CONFLICT	GB 12002892
A	51	ALA	THR	CONFLICT	GB 12002892
A	53	THR	ARG	CONFLICT	GB 12002892
A	84	ALA	VAL	CONFLICT	GB 12002892
A	96	TYR	PRO	CONFLICT	GB 12002892
A	99	GLY	-	INSERTION	GB 12002892
A	102	THR	SER	CONFLICT	GB 12002892
A	103	LYS	ALA	CONFLICT	GB 12002892
A	104	LEU	PRO	CONFLICT	GB 12002892
A	105	GLU	SER	CONFLICT	GB 12002892
A	106	ILE	CYS	CONFLICT	GB 12002892
A	107	LEU	LYS	CONFLICT	GB 12002892
A	?	-	VAL	DELETION	GB 12002892
C	28	GLU	ASP	CONFLICT	GB 12002892
C	30	SER	GLY	CONFLICT	GB 12002892
C	31	GLY	VAL	CONFLICT	GB 12002892
C	32	TYR	SER	CONFLICT	GB 12002892

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	34	SER	ASN	CONFLICT	GB 12002892
C	39	LYS	GLU	CONFLICT	GB 12002892
C	50	ALA	GLY	CONFLICT	GB 12002892
C	51	ALA	THR	CONFLICT	GB 12002892
C	53	THR	ARG	CONFLICT	GB 12002892
C	84	ALA	VAL	CONFLICT	GB 12002892
C	96	TYR	PRO	CONFLICT	GB 12002892
C	99	GLY	-	INSERTION	GB 12002892
C	102	THR	SER	CONFLICT	GB 12002892
C	103	LYS	ALA	CONFLICT	GB 12002892
C	104	LEU	PRO	CONFLICT	GB 12002892
C	105	GLU	SER	CONFLICT	GB 12002892
C	106	ILE	CYS	CONFLICT	GB 12002892
C	107	LEU	LYS	CONFLICT	GB 12002892
C	?	-	VAL	DELETION	GB 12002892
E	28	GLU	ASP	CONFLICT	GB 12002892
E	30	SER	GLY	CONFLICT	GB 12002892
E	31	GLY	VAL	CONFLICT	GB 12002892
E	32	TYR	SER	CONFLICT	GB 12002892
E	34	SER	ASN	CONFLICT	GB 12002892
E	39	LYS	GLU	CONFLICT	GB 12002892
E	50	ALA	GLY	CONFLICT	GB 12002892
E	51	ALA	THR	CONFLICT	GB 12002892
E	53	THR	ARG	CONFLICT	GB 12002892
E	84	ALA	VAL	CONFLICT	GB 12002892
E	96	TYR	PRO	CONFLICT	GB 12002892
E	99	GLY	-	INSERTION	GB 12002892
E	102	THR	SER	CONFLICT	GB 12002892
E	103	LYS	ALA	CONFLICT	GB 12002892
E	104	LEU	PRO	CONFLICT	GB 12002892
E	105	GLU	SER	CONFLICT	GB 12002892
E	106	ILE	CYS	CONFLICT	GB 12002892
E	107	LEU	LYS	CONFLICT	GB 12002892
E	?	-	VAL	DELETION	GB 12002892

- Molecule 2 is a protein called IGG2A FAB FRAGMENT CNJ206.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	220	1647	1039	275	325	8	0	0	0
			Total	C	N	O	S			
2	D	220	1647	1039	275	325	8	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	220	1647	1039	275	325	8	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	GLN	LYS	CONFLICT	GB 4091056
B	18	ARG	LEU	CONFLICT	GB 4091056
B	30	SER	ARG	CONFLICT	GB 4091056
B	32	PHE	HIS	CONFLICT	GB 4091056
B	33	GLY	ALA	CONFLICT	GB 4091056
B	35	HIS	SER	CONFLICT	GB 4091056
B	40	ALA	SER	CONFLICT	GB 4091056
B	44	GLY	ARG	CONFLICT	GB 4091056
B	50	TYR	GLU	CONFLICT	GB 4091056
B	?	-	ASN	DELETION	GB 4091056
B	52	SER	THR	CONFLICT	GB 4091056
B	55	SER	THR	CONFLICT	GB 4091056
B	56	SER	TYR	CONFLICT	GB 4091056
B	58	ILE	-	INSERTION	GB 4091056
B	59	TYR	PHE	CONFLICT	GB 4091056
B	61	ALA	SER	CONFLICT	GB 4091056
B	65	LYS	THR	CONFLICT	GB 4091056
B	75	PRO	ALA	CONFLICT	GB 4091056
B	80	PHE	TYR	CONFLICT	GB 4091056
B	82	GLN	GLU	CONFLICT	GB 4091056
B	84	THR	SER	CONFLICT	GB 4091056
B	99	GLY	-	INSERTION	GB 4091056
B	101	TYR	GLY	CONFLICT	GB 4091056
B	102	TYR	SER	CONFLICT	GB 4091056
B	103	GLY	SER	CONFLICT	GB 4091056
B	105	ARG	SER	CONFLICT	GB 4091056
B	106	GLY	PHE	CONFLICT	GB 4091056
B	107	ALA	VAL	CONFLICT	GB 4091056
D	13	GLN	LYS	CONFLICT	GB 4091056
D	18	ARG	LEU	CONFLICT	GB 4091056
D	30	SER	ARG	CONFLICT	GB 4091056
D	32	PHE	HIS	CONFLICT	GB 4091056
D	33	GLY	ALA	CONFLICT	GB 4091056
D	35	HIS	SER	CONFLICT	GB 4091056
D	40	ALA	SER	CONFLICT	GB 4091056
D	44	GLY	ARG	CONFLICT	GB 4091056

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	50	TYR	GLU	CONFLICT	GB 4091056
D	?	-	ASN	DELETION	GB 4091056
D	52	SER	THR	CONFLICT	GB 4091056
D	55	SER	THR	CONFLICT	GB 4091056
D	56	SER	TYR	CONFLICT	GB 4091056
D	58	ILE	-	INSERTION	GB 4091056
D	59	TYR	PHE	CONFLICT	GB 4091056
D	61	ALA	SER	CONFLICT	GB 4091056
D	65	LYS	THR	CONFLICT	GB 4091056
D	75	PRO	ALA	CONFLICT	GB 4091056
D	80	PHE	TYR	CONFLICT	GB 4091056
D	82	GLN	GLU	CONFLICT	GB 4091056
D	84	THR	SER	CONFLICT	GB 4091056
D	99	GLY	-	INSERTION	GB 4091056
D	101	TYR	GLY	CONFLICT	GB 4091056
D	102	TYR	SER	CONFLICT	GB 4091056
D	103	GLY	SER	CONFLICT	GB 4091056
D	105	ARG	SER	CONFLICT	GB 4091056
D	106	GLY	PHE	CONFLICT	GB 4091056
D	107	ALA	VAL	CONFLICT	GB 4091056
F	13	GLN	LYS	CONFLICT	GB 4091056
F	18	ARG	LEU	CONFLICT	GB 4091056
F	30	SER	ARG	CONFLICT	GB 4091056
F	32	PHE	HIS	CONFLICT	GB 4091056
F	33	GLY	ALA	CONFLICT	GB 4091056
F	35	HIS	SER	CONFLICT	GB 4091056
F	40	ALA	SER	CONFLICT	GB 4091056
F	44	GLY	ARG	CONFLICT	GB 4091056
F	50	TYR	GLU	CONFLICT	GB 4091056
F	?	-	ASN	DELETION	GB 4091056
F	52	SER	THR	CONFLICT	GB 4091056
F	55	SER	THR	CONFLICT	GB 4091056
F	56	SER	TYR	CONFLICT	GB 4091056
F	58	ILE	-	INSERTION	GB 4091056
F	59	TYR	PHE	CONFLICT	GB 4091056
F	61	ALA	SER	CONFLICT	GB 4091056
F	65	LYS	THR	CONFLICT	GB 4091056
F	75	PRO	ALA	CONFLICT	GB 4091056
F	80	PHE	TYR	CONFLICT	GB 4091056
F	82	GLN	GLU	CONFLICT	GB 4091056
F	84	THR	SER	CONFLICT	GB 4091056
F	99	GLY	-	INSERTION	GB 4091056

Continued on next page...

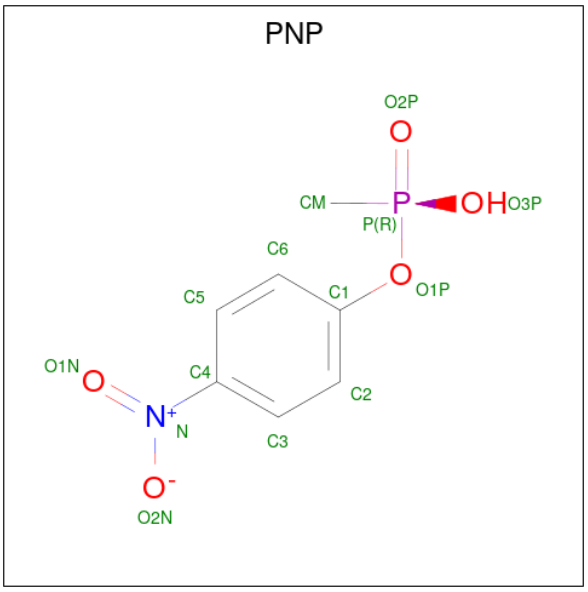
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	101	TYR	GLY	CONFLICT	GB 4091056
F	102	TYR	SER	CONFLICT	GB 4091056
F	103	GLY	SER	CONFLICT	GB 4091056
F	105	ARG	SER	CONFLICT	GB 4091056
F	106	GLY	PHE	CONFLICT	GB 4091056
F	107	ALA	VAL	CONFLICT	GB 4091056

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

- Molecule 4 is METHYL-PHOSPHONIC ACID MONO-(4-NITRO-PHENYL) ESTER (three-letter code: PNP) (formula: $C_7H_8NO_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	14	7	1	5	1	0	0
			Total	C	N	O	P		
4	D	1	14	7	1	5	1	0	0
			Total	C	N	O	P		
4	F	1	14	7	1	5	1	0	0

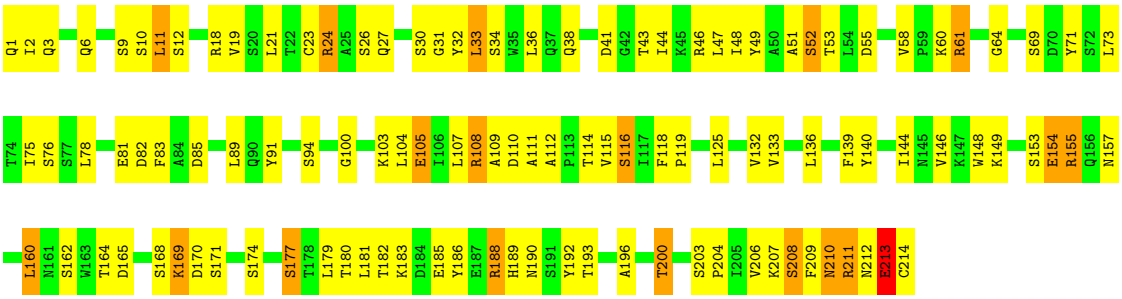
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

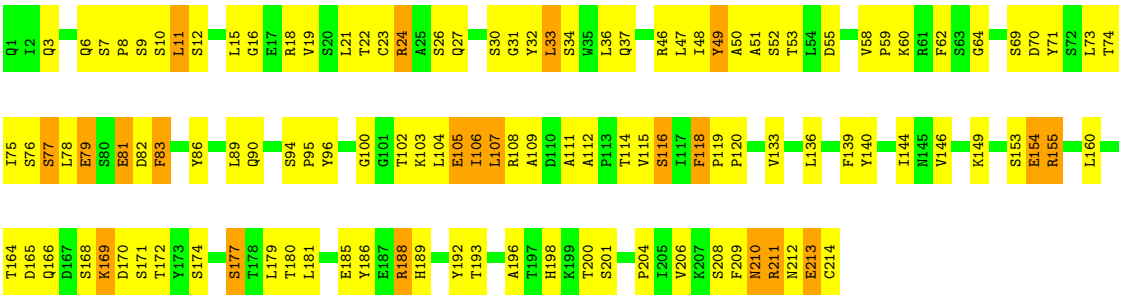
• Molecule 1: IGG2A FAB FRAGMENT CNJ206

Chain A: 47% 44% 8%



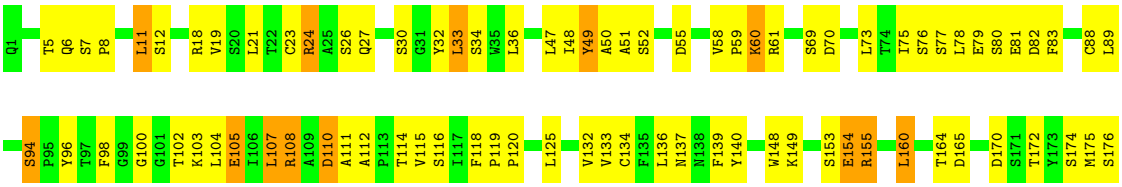
• Molecule 1: IGG2A FAB FRAGMENT CNJ206

Chain C: 45% 45% 10%



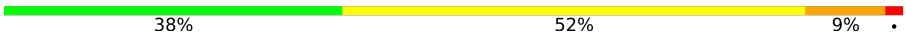
• Molecule 1: IGG2A FAB FRAGMENT CNJ206

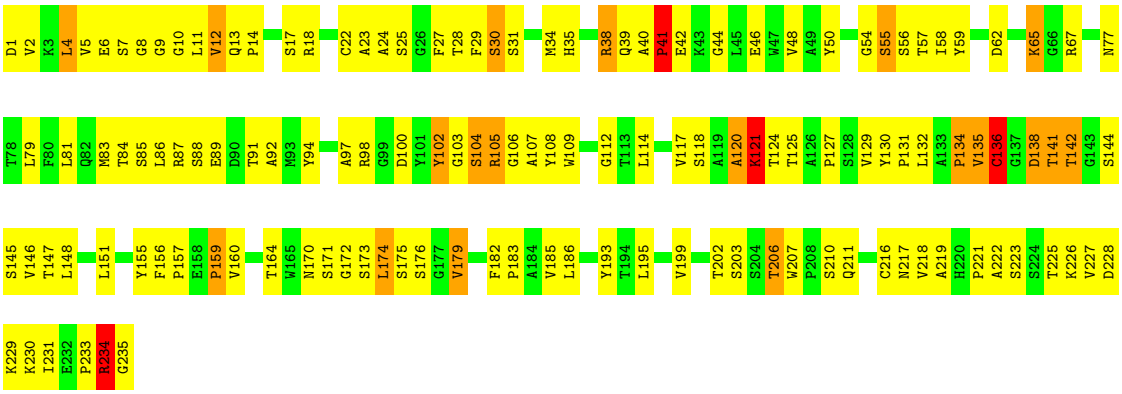
Chain E: 50% 43% 8%



• Molecule 2: IGG2A FAB FRAGMENT CNJ206

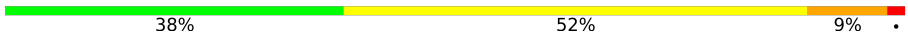
Chain B:

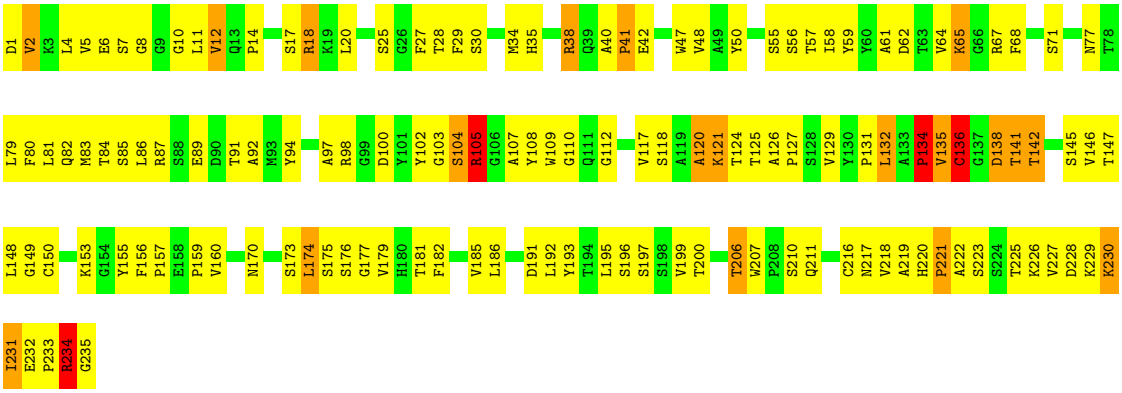




• Molecule 2: IGG2A FAB FRAGMENT CNJ206

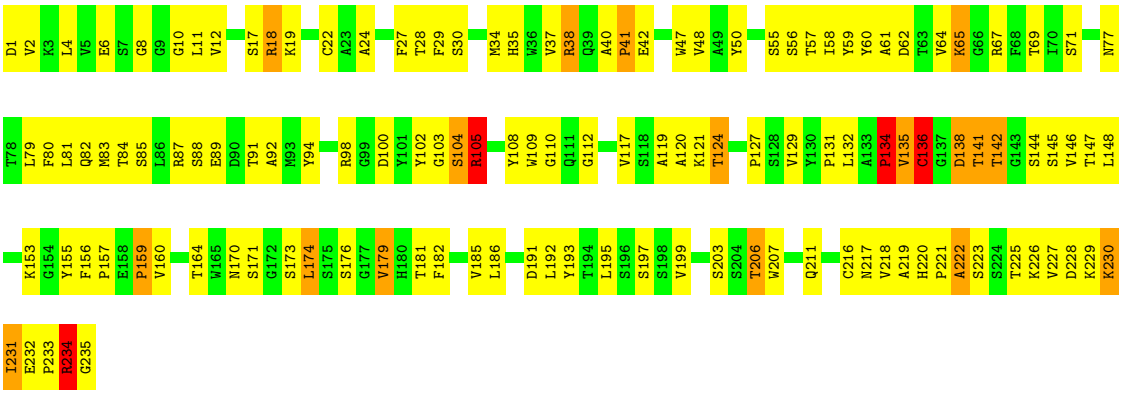
Chain D:





• Molecule 2: IGG2A FAB FRAGMENT CNJ206

Chain F:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	74.10Å 76.90Å 88.30Å 93.80° 93.90° 115.60°	Depositor
Resolution (Å)	7.00 – 3.20	Depositor
% Data completeness (in resolution range)	96.0 (7.00-3.20)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.200 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9949	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.67	0/1689	0.90	0/2288
1	C	0.69	1/1689 (0.1%)	0.89	0/2288
1	E	0.66	0/1689	0.91	4/2288 (0.2%)
2	B	0.68	0/1689	0.87	0/2301
2	D	0.65	0/1689	0.84	0/2301
2	F	0.67	0/1689	0.85	0/2301
All	All	0.67	1/10134 (0.0%)	0.88	4/13767 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	79	GLU	CG-CD	5.52	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	107	LEU	CA-CB-CG	5.42	127.77	115.30
1	E	160	LEU	CA-CB-CG	5.19	127.23	115.30
1	E	137	ASN	N-CA-C	5.08	124.72	111.00
1	E	110	ASP	CA-C-O	5.04	130.69	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1655	0	1586	100	1
1	C	1655	0	1586	110	1
1	E	1655	0	1586	91	0
2	B	1647	0	1605	127	0
2	D	1647	0	1605	142	0
2	F	1647	0	1605	103	0
3	A	1	0	0	0	0
4	B	14	0	7	2	0
4	D	14	0	7	4	0
4	F	14	0	7	3	0
All	All	9949	0	9594	633	1

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 32.

All (633) 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:C:108:ARG:HD3	1:C:171:SER:HB2	1.25	1.19
2:D:62:ASP:HA	2:D:65:LYS:HD3	1.38	1.03
2:F:127:PRO:HB3	2:F:155:TYR:HB3	1.44	1.00
2:B:127:PRO:HB3	2:B:155:TYR:HB3	1.44	0.99
1:A:108:ARG:HD2	1:A:171:SER:HB2	1.46	0.98
2:D:127:PRO:HB3	2:D:155:TYR:HB3	1.46	0.97
2:D:135:VAL:HG13	2:D:136:CYS:SG	2.05	0.95
2:B:62:ASP:HA	2:B:65:LYS:HD3	1.47	0.95
2:F:135:VAL:HG13	2:F:136:CYS:SG	2.07	0.94
2:B:135:VAL:HG13	2:B:136:CYS:SG	2.08	0.93
2:F:62:ASP:HA	2:F:65:LYS:HD3	1.50	0.92
2:D:179:VAL:HG12	2:D:199:VAL:HG23	1.57	0.87
1:C:185:GLU:HG2	1:C:188:ARG:HE	1.44	0.81
2:D:62:ASP:HA	2:D:65:LYS:CD	2.09	0.81
1:A:185:GLU:HG2	1:A:188:ARG:HE	1.45	0.81
1:A:185:GLU:HA	1:A:188:ARG:HG2	1.63	0.81
2:D:105:ARG:HG3	2:D:105:ARG:HH11	1.47	0.79
2:D:141:THR:HG21	2:D:147:THR:HG21	1.64	0.79
1:A:118:PHE:CD2	2:B:132:LEU:HB3	2.17	0.79
2:D:207:TRP:CZ2	2:D:233:PRO:HG3	2.18	0.79
1:E:108:ARG:HH11	1:E:108:ARG:HG3	1.48	0.78
1:C:108:ARG:HG2	1:C:109:ALA:H	1.48	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:207:TRP:CZ2	2:F:233:PRO:HG3	2.19	0.78
1:E:18:ARG:HG3	1:E:76:SER:HA	1.64	0.78
1:A:24:ARG:HH12	1:A:69:SER:HB2	1.50	0.77
1:C:112:ALA:N	1:C:200:THR:HG21	1.99	0.77
2:D:67:ARG:HB3	2:D:84:THR:O	1.85	0.77
1:E:185:GLU:HG2	1:E:188:ARG:HE	1.50	0.77
2:D:142:THR:HB	2:D:145:SER:OG	1.86	0.76
2:F:38:ARG:HG2	2:F:48:VAL:CG2	2.15	0.76
1:A:112:ALA:N	1:A:200:THR:HG21	2.01	0.76
1:C:118:PHE:CD2	2:D:132:LEU:HB3	2.20	0.76
1:C:24:ARG:HH12	1:C:69:SER:HB2	1.49	0.76
1:E:185:GLU:HA	1:E:188:ARG:HG2	1.67	0.76
1:C:185:GLU:HA	1:C:188:ARG:HG2	1.66	0.75
1:E:11:LEU:HG	1:E:104:LEU:HD12	1.66	0.75
2:F:38:ARG:HG2	2:F:48:VAL:HG21	1.68	0.75
2:B:142:THR:HB	2:B:145:SER:OG	1.86	0.75
2:F:17:SER:OG	2:F:84:THR:HA	1.87	0.75
1:A:18:ARG:HG3	1:A:76:SER:HA	1.67	0.75
1:E:26:SER:O	1:E:27:GLN:HG3	1.88	0.74
2:B:67:ARG:HB3	2:B:84:THR:O	1.87	0.74
2:D:2:VAL:HG21	2:D:108:TYR:CD2	2.22	0.74
2:D:2:VAL:HG11	2:D:108:TYR:CE1	2.23	0.74
2:B:87:ARG:HG3	2:B:87:ARG:HH11	1.53	0.74
2:B:141:THR:HG21	2:B:147:THR:HG21	1.69	0.74
2:F:67:ARG:HB3	2:F:84:THR:O	1.87	0.74
1:C:11:LEU:HG	1:C:104:LEU:HD12	1.67	0.73
1:E:6:GLN:HB2	1:E:23:CYS:SG	2.27	0.73
1:E:193:THR:HA	1:E:208:SER:HB3	1.71	0.73
2:F:156:PHE:CE1	2:F:157:PRO:HB3	2.24	0.73
2:B:207:TRP:CZ2	2:B:233:PRO:HG3	2.23	0.73
1:C:18:ARG:HG3	1:C:76:SER:HA	1.69	0.73
2:D:87:ARG:HG3	2:D:87:ARG:HH11	1.53	0.72
1:E:112:ALA:N	1:E:200:THR:HG21	2.04	0.72
2:D:2:VAL:HG11	2:D:108:TYR:CZ	2.24	0.72
2:B:2:VAL:HG11	2:B:108:TYR:CE1	2.24	0.72
1:C:83:PHE:HB2	1:C:106:ILE:HD11	1.72	0.71
2:D:10:GLY:HA3	2:D:18:ARG:NH2	2.05	0.71
2:B:2:VAL:HG21	2:B:108:TYR:CD2	2.25	0.71
1:A:11:LEU:HG	1:A:104:LEU:HD12	1.74	0.70
2:D:35:HIS:CE1	2:D:50:TYR:CD1	2.79	0.70
2:B:2:VAL:HG11	2:B:108:TYR:CZ	2.26	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10:GLY:HA3	2:F:18:ARG:NH2	2.06	0.70
2:B:10:GLY:HA3	2:B:18:ARG:NH2	2.07	0.70
1:C:108:ARG:CD	1:C:171:SER:HB2	2.15	0.69
2:D:216:CYS:O	2:D:228:ASP:HA	1.93	0.69
2:F:2:VAL:HG11	2:F:108:TYR:CE1	2.28	0.69
2:D:135:VAL:HG13	2:D:136:CYS:HG	1.57	0.69
2:F:11:LEU:HD12	2:F:157:PRO:HD3	1.75	0.69
2:D:141:THR:HG21	2:D:147:THR:CG2	2.22	0.68
1:E:47:LEU:HA	1:E:58:VAL:HG21	1.74	0.68
2:D:233:PRO:O	2:D:234:ARG:HB2	1.93	0.68
1:E:160:LEU:HD11	2:F:185:VAL:HB	1.76	0.68
2:F:141:THR:HG21	2:F:147:THR:HG21	1.74	0.68
2:D:219:ALA:O	2:D:221:PRO:HD3	1.95	0.67
2:D:179:VAL:HG12	2:D:199:VAL:CG2	2.24	0.67
2:D:186:LEU:HD12	2:D:192:LEU:O	1.95	0.67
2:F:135:VAL:O	2:F:136:CYS:SG	2.53	0.67
1:C:33:LEU:HD22	1:C:89:LEU:O	1.95	0.66
2:D:135:VAL:C	2:D:136:CYS:SG	2.73	0.66
1:C:136:LEU:HD21	1:C:196:ALA:HB2	1.77	0.66
1:C:160:LEU:HD11	2:D:185:VAL:HB	1.76	0.66
2:B:35:HIS:CE1	2:B:50:TYR:CD1	2.83	0.66
1:E:79:GLU:HB2	1:E:81:GLU:OE1	1.96	0.66
2:F:62:ASP:HA	2:F:65:LYS:CD	2.25	0.66
2:D:38:ARG:HG2	2:D:48:VAL:CG2	2.26	0.65
2:F:2:VAL:HG11	2:F:108:TYR:CZ	2.31	0.65
1:E:21:LEU:HD22	1:E:102:THR:HG21	1.77	0.65
1:A:114:THR:HG22	2:B:141:THR:HG22	1.79	0.65
1:C:193:THR:HA	1:C:208:SER:HB3	1.78	0.65
2:F:87:ARG:HG3	2:F:87:ARG:HH11	1.61	0.65
1:A:108:ARG:CD	1:A:171:SER:HB2	2.25	0.65
2:D:2:VAL:HG11	2:D:108:TYR:CD1	2.31	0.65
2:D:105:ARG:HH11	2:D:105:ARG:CG	2.09	0.65
2:F:2:VAL:HG11	2:F:108:TYR:CD1	2.32	0.64
2:B:2:VAL:HG11	2:B:108:TYR:CD1	2.32	0.64
1:E:48:ILE:HD12	1:E:73:LEU:HD13	1.79	0.64
1:C:24:ARG:NH1	1:C:69:SER:HB2	2.12	0.64
2:F:142:THR:HB	2:F:145:SER:OG	1.97	0.64
2:B:134:PRO:HD3	2:B:148:LEU:HG	1.79	0.64
2:D:134:PRO:HD3	2:D:148:LEU:HG	1.80	0.64
1:A:11:LEU:HD21	1:A:19:VAL:CG1	2.28	0.63
2:F:141:THR:HG21	2:F:147:THR:CG2	2.27	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD12	1:A:140:TYR:OH	1.98	0.63
1:A:12:SER:HA	1:A:105:GLU:O	1.98	0.63
2:B:147:THR:C	2:B:148:LEU:HD12	2.19	0.63
1:C:6:GLN:HB3	1:C:100:GLY:H	1.64	0.63
2:F:105:ARG:HH11	2:F:105:ARG:CG	2.12	0.63
1:C:168:SER:OG	1:C:169:LYS:HE2	1.99	0.62
2:B:34:MET:SD	2:B:98:ARG:HA	2.39	0.62
2:B:141:THR:HG21	2:B:147:THR:CG2	2.30	0.62
2:D:6:GLU:OE2	2:D:110:GLY:HA3	2.00	0.62
1:A:24:ARG:NH1	1:A:69:SER:HB2	2.14	0.62
1:E:6:GLN:HB3	1:E:100:GLY:H	1.65	0.62
1:C:26:SER:O	1:C:27:GLN:HG3	1.99	0.62
1:C:47:LEU:HA	1:C:58:VAL:HG21	1.82	0.62
2:D:35:HIS:CE1	2:D:50:TYR:HD1	2.18	0.62
2:B:216:CYS:O	2:B:228:ASP:HA	1.99	0.62
1:E:108:ARG:HG3	1:E:108:ARG:NH1	2.15	0.62
2:F:2:VAL:HG21	2:F:108:TYR:CD2	2.35	0.61
2:D:87:ARG:HD3	2:D:89:GLU:OE1	2.00	0.61
2:B:62:ASP:HA	2:B:65:LYS:CD	2.26	0.61
1:A:47:LEU:HA	1:A:58:VAL:HG21	1.81	0.61
2:F:11:LEU:HD11	2:F:156:PHE:HE1	1.66	0.60
1:A:193:THR:HA	1:A:208:SER:HB3	1.82	0.60
1:A:180:THR:O	1:A:181:LEU:HD23	2.01	0.60
1:C:115:VAL:HG22	1:C:136:LEU:HG	1.83	0.60
2:D:2:VAL:HG11	2:D:108:TYR:CE2	2.36	0.60
1:C:11:LEU:HD21	1:C:19:VAL:HG13	1.84	0.60
2:B:135:VAL:HG13	2:B:136:CYS:HG	1.66	0.60
1:E:155:ARG:HD2	1:E:179:LEU:HD11	1.84	0.60
1:E:174:SER:HB3	2:F:182:PHE:HE1	1.67	0.60
1:A:132:VAL:HG12	1:A:148:TRP:HH2	1.67	0.59
2:D:131:PRO:HD3	2:D:229:LYS:HG2	1.83	0.59
2:F:216:CYS:O	2:F:228:ASP:HA	2.01	0.59
2:B:5:VAL:HG12	2:B:5:VAL:O	2.02	0.59
1:E:108:ARG:NH2	1:E:111:ALA:HB2	2.17	0.59
2:D:10:GLY:HA3	2:D:18:ARG:HH21	1.66	0.59
2:B:2:VAL:HG11	2:B:108:TYR:CE2	2.38	0.59
2:D:156:PHE:CE1	2:D:157:PRO:HB3	2.38	0.59
1:E:164:THR:HG22	1:E:165:ASP:N	2.17	0.59
1:E:118:PHE:CD2	2:F:132:LEU:HB3	2.38	0.59
1:E:103:LYS:HD2	1:E:103:LYS:N	2.18	0.59
2:F:233:PRO:O	2:F:234:ARG:HB2	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:MET:SD	2:D:98:ARG:HA	2.43	0.59
2:F:6:GLU:OE2	2:F:110:GLY:HA3	2.03	0.59
2:B:134:PRO:C	2:B:136:CYS:H	2.07	0.58
1:C:33:LEU:HD13	1:C:34:SER:N	2.17	0.58
1:C:114:THR:HG22	2:D:141:THR:HG22	1.85	0.58
1:C:12:SER:HA	1:C:105:GLU:O	2.03	0.58
2:F:2:VAL:HG11	2:F:108:TYR:CE2	2.38	0.58
2:B:38:ARG:HG2	2:B:48:VAL:CG2	2.33	0.58
1:A:119:PRO:HG3	1:A:209:PHE:CG	2.39	0.58
2:D:62:ASP:HA	2:D:65:LYS:CE	2.33	0.58
1:A:211:ARG:O	1:A:212:ASN:HB2	2.03	0.58
1:C:11:LEU:HG	1:C:104:LEU:CD1	2.33	0.58
1:C:11:LEU:HD21	1:C:19:VAL:CG1	2.33	0.58
1:E:213:GLU:O	1:E:214:CYS:HB2	2.04	0.58
1:A:186:TYR:HD1	1:A:192:TYR:CZ	2.22	0.58
2:F:219:ALA:O	2:F:221:PRO:HD3	2.03	0.58
2:D:2:VAL:HA	2:D:25:SER:O	2.04	0.58
2:B:135:VAL:C	2:B:136:CYS:SG	2.82	0.57
1:C:49:TYR:CE1	1:C:53:THR:HB	2.39	0.57
1:E:114:THR:HG22	2:F:141:THR:HG22	1.86	0.57
2:B:12:VAL:O	2:B:117:VAL:HA	2.04	0.57
2:D:135:VAL:O	2:D:136:CYS:SG	2.62	0.57
1:A:146:VAL:HG11	1:A:177:SER:OG	2.05	0.57
2:B:125:THR:O	2:B:155:TYR:HA	2.05	0.57
2:B:134:PRO:O	2:B:136:CYS:N	2.37	0.57
1:E:115:VAL:HG22	1:E:136:LEU:HG	1.85	0.57
1:E:211:ARG:O	1:E:212:ASN:HB2	2.04	0.57
2:D:103:GLY:O	2:D:105:ARG:N	2.37	0.57
2:F:147:THR:C	2:F:148:LEU:HD12	2.23	0.57
1:A:118:PHE:HD2	2:B:132:LEU:HB3	1.70	0.57
1:C:213:GLU:O	1:C:214:CYS:HB2	2.05	0.57
1:A:108:ARG:HH11	1:A:108:ARG:HB3	1.70	0.57
1:A:185:GLU:HG2	1:A:188:ARG:NE	2.19	0.57
1:A:19:VAL:HG21	1:A:78:LEU:HD11	1.87	0.57
1:C:108:ARG:HG2	1:C:108:ARG:HH11	1.70	0.57
1:C:36:LEU:HD11	2:D:109:TRP:CZ2	2.39	0.57
2:F:35:HIS:CE1	2:F:50:TYR:CD1	2.93	0.56
1:A:81:GLU:HG3	1:E:81:GLU:OE2	2.06	0.56
1:A:108:ARG:NH1	1:A:109:ALA:O	2.38	0.56
2:D:148:LEU:HD23	2:D:231:ILE:HG21	1.86	0.56
1:E:120:PRO:HD2	1:E:186:TYR:OH	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:24:ALA:HB1	2:F:27:PHE:CE1	2.41	0.56
2:F:134:PRO:O	2:F:135:VAL:HG12	2.06	0.56
1:A:18:ARG:HG3	1:A:75:ILE:O	2.04	0.56
1:C:19:VAL:HG21	1:C:78:LEU:HD11	1.86	0.56
2:D:104:SER:O	2:D:105:ARG:HB3	2.06	0.56
2:F:179:VAL:HG12	2:F:199:VAL:HG23	1.86	0.56
1:A:108:ARG:HD2	1:A:170:ASP:O	2.06	0.56
1:C:108:ARG:HH21	1:C:172:THR:HG22	1.71	0.56
1:A:136:LEU:HD21	1:A:196:ALA:HB2	1.87	0.55
2:D:48:VAL:HA	2:D:61:ALA:HB2	1.88	0.55
2:F:17:SER:HB3	2:F:83:MET:O	2.06	0.55
2:F:135:VAL:C	2:F:136:CYS:SG	2.85	0.55
1:A:193:THR:OG1	1:A:208:SER:HB3	2.07	0.55
2:B:146:VAL:HG13	2:B:146:VAL:O	2.07	0.55
1:C:73:LEU:HD12	1:C:74:THR:N	2.21	0.55
1:A:179:LEU:HD21	1:A:181:LEU:HD21	1.88	0.55
1:A:204:PRO:O	1:A:206:VAL:HG23	2.06	0.55
2:B:102:TYR:CE1	4:B:551:PNP:CM	2.90	0.55
2:F:134:PRO:HD3	2:F:148:LEU:HG	1.88	0.55
2:D:82:GLN:HE21	2:D:83:MET:N	2.04	0.55
2:D:121:LYS:HG2	2:D:125:THR:OG1	2.07	0.55
2:B:120:ALA:O	2:B:121:LYS:HB3	2.07	0.55
2:B:155:TYR:CE1	2:B:193:TYR:HB2	2.41	0.55
1:C:164:THR:HG22	1:C:165:ASP:N	2.22	0.54
2:D:148:LEU:HD23	2:D:231:ILE:CG2	2.37	0.54
1:E:33:LEU:HD13	1:E:34:SER:N	2.21	0.54
1:E:96:TYR:HD2	2:F:47:TRP:CE2	2.25	0.54
2:F:11:LEU:HD11	2:F:156:PHE:CE1	2.42	0.54
2:B:17:SER:OG	2:B:84:THR:HA	2.08	0.54
1:C:81:GLU:HG3	1:C:82:ASP:OD1	2.07	0.54
1:C:136:LEU:HD21	1:C:196:ALA:CB	2.38	0.54
2:F:2:VAL:HG11	2:F:108:TYR:CG	2.42	0.54
2:F:34:MET:SD	2:F:98:ARG:HA	2.47	0.54
1:C:21:LEU:HD23	1:C:21:LEU:N	2.22	0.54
1:C:133:VAL:HB	2:D:132:LEU:HD11	1.89	0.54
1:C:211:ARG:O	1:C:212:ASN:HB2	2.08	0.54
2:B:38:ARG:HG2	2:B:48:VAL:HG21	1.90	0.54
2:B:11:LEU:HD12	2:B:157:PRO:HD3	1.90	0.54
1:C:108:ARG:HG2	1:C:109:ALA:N	2.20	0.54
1:A:60:LYS:N	1:A:60:LYS:HD2	2.23	0.54
2:B:219:ALA:O	2:B:221:PRO:HD3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:TYR:HE2	2:D:102:TYR:CZ	2.26	0.54
2:D:134:PRO:O	2:D:135:VAL:HG12	2.07	0.54
2:F:100:ASP:O	2:F:104:SER:HB3	2.08	0.54
1:C:185:GLU:OE2	1:C:189:HIS:NE2	2.41	0.53
2:D:97:ALA:HB2	2:D:109:TRP:CE3	2.43	0.53
2:F:2:VAL:HG11	2:F:108:TYR:CD2	2.43	0.53
1:A:11:LEU:HD21	1:A:19:VAL:HG13	1.91	0.53
1:E:136:LEU:HD21	1:E:196:ALA:HB2	1.89	0.53
1:A:213:GLU:O	1:A:214:CYS:HB2	2.08	0.53
1:C:103:LYS:HD2	1:C:103:LYS:N	2.24	0.53
2:D:38:ARG:HG2	2:D:48:VAL:HG21	1.90	0.53
2:D:12:VAL:O	2:D:117:VAL:HA	2.09	0.53
2:B:135:VAL:O	2:B:136:CYS:SG	2.66	0.53
1:C:6:GLN:HB2	1:C:23:CYS:SG	2.48	0.53
1:E:170:ASP:O	1:E:172:THR:HG23	2.09	0.53
2:F:87:ARG:HD3	2:F:89:GLU:OE1	2.08	0.53
2:F:103:GLY:O	2:F:105:ARG:N	2.40	0.53
2:B:83:MET:HE1	2:B:94:TYR:CE2	2.44	0.53
2:D:147:THR:C	2:D:148:LEU:HD12	2.29	0.53
2:F:61:ALA:HB3	2:F:64:VAL:HG22	1.90	0.53
2:F:127:PRO:CB	2:F:155:TYR:HB3	2.30	0.53
1:A:149:LYS:HG2	1:A:154:GLU:HA	1.91	0.52
2:B:234:ARG:HA	2:B:234:ARG:NE	2.24	0.52
2:D:2:VAL:HG11	2:D:108:TYR:CG	2.43	0.52
1:A:6:GLN:HB2	1:A:23:CYS:SG	2.49	0.52
2:D:62:ASP:O	2:D:65:LYS:HE3	2.10	0.52
2:D:134:PRO:O	2:D:136:CYS:N	2.43	0.52
1:C:155:ARG:HD2	1:C:179:LEU:HD11	1.91	0.52
2:D:2:VAL:HG11	2:D:108:TYR:CD2	2.45	0.52
1:E:204:PRO:O	1:E:206:VAL:HG23	2.10	0.52
1:A:160:LEU:HD11	2:B:185:VAL:HB	1.89	0.52
2:B:127:PRO:CB	2:B:155:TYR:HB3	2.31	0.52
2:D:11:LEU:HD12	2:D:157:PRO:HG3	1.91	0.52
2:B:10:GLY:HA3	2:B:18:ARG:HH21	1.73	0.52
1:C:179:LEU:HD21	1:C:181:LEU:HD21	1.92	0.52
2:B:228:ASP:O	2:B:229:LYS:HD2	2.09	0.52
1:C:32:TYR:HE2	2:D:102:TYR:CE2	2.28	0.51
2:D:179:VAL:HA	2:D:199:VAL:HA	1.92	0.51
2:B:35:HIS:CE1	2:B:50:TYR:HD1	2.27	0.51
2:B:40:ALA:O	2:B:42:GLU:N	2.43	0.51
2:F:71:SER:O	2:F:80:PHE:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:HD2	1:A:179:LEU:HD11	1.92	0.51
1:C:193:THR:OG1	1:C:208:SER:HB3	2.11	0.51
2:D:87:ARG:O	2:D:117:VAL:HG11	2.09	0.51
1:C:16:GLY:O	1:C:77:SER:HA	2.11	0.51
1:C:89:LEU:HD12	1:C:90:GLN:N	2.25	0.51
1:E:182:THR:OG1	1:E:184:ASP:HB2	2.10	0.51
2:D:40:ALA:O	2:D:42:GLU:N	2.44	0.51
1:E:11:LEU:HG	1:E:104:LEU:CD1	2.37	0.51
1:E:89:LEU:HD13	1:E:98:PHE:CE1	2.46	0.51
1:A:48:ILE:HD12	1:A:73:LEU:HD13	1.92	0.51
1:A:75:ILE:HG21	1:A:78:LEU:HD23	1.92	0.51
1:A:119:PRO:HG3	1:A:209:PHE:CD2	2.46	0.51
1:E:32:TYR:HE2	2:F:102:TYR:CZ	2.29	0.51
2:B:2:VAL:HG11	2:B:108:TYR:CG	2.46	0.51
1:E:32:TYR:HE2	2:F:102:TYR:CE2	2.29	0.50
1:A:18:ARG:CG	1:A:76:SER:HA	2.38	0.50
2:D:147:THR:HG22	2:D:200:THR:OG1	2.11	0.50
2:D:219:ALA:HB2	2:D:226:LYS:HG2	1.94	0.50
1:E:179:LEU:HD21	1:E:181:LEU:HD21	1.93	0.50
2:F:134:PRO:C	2:F:136:CYS:H	2.15	0.50
2:B:129:VAL:HB	2:B:229:LYS:HD3	1.93	0.50
1:A:168:SER:OG	1:A:169:LYS:HE2	2.09	0.50
2:B:87:ARG:O	2:B:117:VAL:HG11	2.10	0.50
2:B:131:PRO:HD3	2:B:229:LYS:HG2	1.92	0.50
1:C:89:LEU:HD12	1:C:90:GLN:H	1.77	0.50
1:C:186:TYR:HD1	1:C:192:TYR:HH	1.59	0.50
1:E:139:PHE:O	1:E:172:THR:HB	2.11	0.50
2:F:134:PRO:HG3	2:F:147:THR:O	2.11	0.50
2:B:29:PHE:CD2	2:B:77:ASN:HA	2.46	0.50
2:B:135:VAL:HB	2:B:235:GLY:OXT	2.11	0.50
2:D:71:SER:O	2:D:80:PHE:N	2.45	0.50
2:D:102:TYR:CE1	4:D:552:PNP:CM	2.95	0.50
1:E:190:ASN:ND2	1:E:210:ASN:HD21	2.10	0.50
1:A:32:TYR:O	1:A:91:TYR:CD1	2.65	0.50
1:A:26:SER:O	1:A:27:GLN:HG3	2.12	0.49
1:A:162:SER:OG	2:B:183:PRO:HG2	2.12	0.49
1:E:24:ARG:HH12	1:E:69:SER:HB2	1.76	0.49
2:F:221:PRO:O	2:F:223:SER:N	2.45	0.49
1:A:186:TYR:HD1	1:A:192:TYR:OH	1.94	0.49
1:C:204:PRO:O	1:C:206:VAL:HG23	2.12	0.49
2:F:29:PHE:CD2	2:F:77:ASN:HA	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:148:LEU:HD23	2:F:231:ILE:HG21	1.93	0.49
2:F:170:ASN:HD22	2:F:174:LEU:HB2	1.77	0.49
2:B:179:VAL:HA	2:B:199:VAL:HA	1.93	0.49
1:C:106:ILE:HG22	1:C:106:ILE:O	2.12	0.49
1:C:146:VAL:HG11	1:C:177:SER:OG	2.11	0.49
1:E:48:ILE:CD1	1:E:73:LEU:HD13	2.40	0.49
1:E:75:ILE:CG2	1:E:78:LEU:HD23	2.42	0.49
1:C:24:ARG:HG3	1:C:70:ASP:OD2	2.13	0.49
1:C:107:LEU:HA	1:C:140:TYR:OH	2.11	0.49
1:E:108:ARG:NH1	1:E:108:ARG:CG	2.76	0.49
2:B:2:VAL:HG11	2:B:108:TYR:CD2	2.48	0.49
2:D:134:PRO:C	2:D:136:CYS:H	2.15	0.49
2:F:12:VAL:O	2:F:117:VAL:HA	2.13	0.49
2:B:41:PRO:O	2:B:42:GLU:HG3	2.13	0.49
2:B:233:PRO:O	2:B:234:ARG:HB2	2.12	0.49
1:C:18:ARG:CG	1:C:76:SER:HA	2.41	0.49
2:D:17:SER:HB3	2:D:83:MET:O	2.13	0.49
1:E:111:ALA:C	1:E:200:THR:HG21	2.33	0.49
1:A:103:LYS:HD2	1:A:103:LYS:N	2.28	0.49
1:A:115:VAL:HG22	1:A:136:LEU:HG	1.94	0.49
2:D:219:ALA:HA	2:D:225:THR:O	2.12	0.49
1:A:11:LEU:HG	1:A:104:LEU:CD1	2.43	0.49
2:B:210:SER:HB2	2:B:211:GLN:OE1	2.13	0.49
1:E:60:LYS:HD2	1:E:60:LYS:N	2.28	0.49
1:A:148:TRP:HE1	1:A:177:SER:HB3	1.76	0.48
2:B:104:SER:O	2:B:105:ARG:HB3	2.13	0.48
2:D:210:SER:HB2	2:D:211:GLN:OE1	2.13	0.48
2:F:60:TYR:OH	2:F:69:THR:HA	2.13	0.48
1:E:89:LEU:HD13	1:E:98:PHE:CD1	2.49	0.48
2:B:17:SER:HB3	2:B:83:MET:O	2.13	0.48
2:B:67:ARG:O	2:B:84:THR:HB	2.14	0.48
2:B:159:PRO:O	2:B:221:PRO:HD2	2.14	0.48
1:C:180:THR:O	1:C:181:LEU:HD23	2.14	0.48
1:E:119:PRO:HG3	1:E:209:PHE:CG	2.49	0.48
2:F:146:VAL:HG13	2:F:146:VAL:O	2.13	0.48
2:F:186:LEU:HD13	2:F:193:TYR:CZ	2.49	0.48
2:B:9:GLY:HA3	2:B:114:LEU:O	2.13	0.48
2:F:186:LEU:HD12	2:F:192:LEU:O	2.12	0.48
1:A:116:SER:HB3	2:B:141:THR:HG23	1.95	0.48
1:E:24:ARG:HG3	1:E:70:ASP:OD2	2.13	0.48
1:E:209:PHE:CD2	1:E:210:ASN:N	2.82	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PHE:CE2	1:A:144:ILE:HB	2.49	0.48
2:D:186:LEU:HA	2:D:192:LEU:O	2.14	0.48
2:B:206:THR:HA	2:B:211:GLN:OE1	2.14	0.48
1:C:19:VAL:CG2	1:C:78:LEU:HD11	2.43	0.48
2:D:105:ARG:HG3	2:D:105:ARG:NH1	2.23	0.48
1:A:33:LEU:HD13	1:A:34:SER:N	2.29	0.47
1:E:18:ARG:HD2	1:E:76:SER:HB3	1.96	0.47
2:B:219:ALA:HA	2:B:225:THR:O	2.14	0.47
1:C:186:TYR:HD1	1:C:192:TYR:CZ	2.31	0.47
2:F:159:PRO:O	2:F:221:PRO:HD2	2.14	0.47
2:B:97:ALA:HB2	2:B:109:TRP:CE3	2.49	0.47
1:C:49:TYR:O	1:C:50:ALA:HB3	2.14	0.47
1:E:61:ARG:NH2	1:E:82:ASP:OD1	2.46	0.47
1:C:111:ALA:O	1:C:139:PHE:HA	2.15	0.47
2:D:177:GLY:O	2:D:199:VAL:HA	2.15	0.47
2:D:185:VAL:O	2:D:193:TYR:HA	2.14	0.47
2:D:64:VAL:O	2:D:65:LYS:C	2.53	0.47
2:B:65:LYS:HE3	2:B:65:LYS:HB2	1.75	0.47
2:B:67:ARG:NH1	2:B:85:SER:O	2.47	0.47
2:B:103:GLY:O	2:B:105:ARG:N	2.47	0.47
2:B:124:THR:CG2	2:B:223:SER:HB3	2.44	0.47
1:C:24:ARG:HA	1:C:69:SER:O	2.15	0.47
2:D:87:ARG:HH11	2:D:87:ARG:CG	2.26	0.47
1:E:12:SER:HA	1:E:105:GLU:O	2.15	0.47
2:F:135:VAL:HB	2:F:235:GLY:OXT	2.14	0.47
2:B:179:VAL:HG12	2:B:199:VAL:HG23	1.96	0.47
2:B:185:VAL:O	2:B:193:TYR:HA	2.14	0.47
2:D:6:GLU:CD	2:D:112:GLY:H	2.17	0.47
1:A:209:PHE:CD2	1:A:210:ASN:N	2.83	0.47
1:E:32:TYR:CE2	2:F:102:TYR:CZ	3.03	0.47
2:B:102:TYR:CD1	4:B:551:PNP:CM	2.98	0.47
1:E:108:ARG:HE	1:E:172:THR:HG22	1.79	0.47
2:F:104:SER:O	2:F:105:ARG:HB3	2.14	0.47
2:F:142:THR:HG22	2:F:144:SER:OG	2.15	0.47
1:C:118:PHE:HD2	2:D:132:LEU:HB3	1.74	0.46
2:D:67:ARG:NH1	2:D:85:SER:O	2.47	0.46
2:B:38:ARG:HD2	2:B:46:GLU:OE1	2.16	0.46
1:E:136:LEU:HD21	1:E:196:ALA:CB	2.45	0.46
1:E:164:THR:HG22	1:E:165:ASP:O	2.15	0.46
2:F:58:ILE:O	2:F:59:TYR:HD1	1.98	0.46
1:A:36:LEU:HD11	2:B:109:TRP:CZ2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:160:VAL:CG2	2:F:218:VAL:HG13	2.45	0.46
1:C:108:ARG:HD3	1:C:171:SER:CB	2.18	0.46
1:A:85:ASP:OD1	1:A:103:LYS:HA	2.16	0.46
2:B:170:ASN:HD22	2:B:174:LEU:HB2	1.80	0.46
1:C:21:LEU:HD22	1:C:102:THR:HG21	1.98	0.46
1:C:81:GLU:HG3	1:C:82:ASP:H	1.81	0.46
1:E:18:ARG:CG	1:E:76:SER:HA	2.39	0.46
1:E:186:TYR:HD1	1:E:192:TYR:CZ	2.33	0.46
1:A:136:LEU:HD21	1:A:196:ALA:CB	2.45	0.46
2:B:87:ARG:HH11	2:B:87:ARG:CG	2.26	0.46
2:B:129:VAL:O	2:B:229:LYS:HE2	2.14	0.46
2:D:118:SER:HG	2:D:156:PHE:HZ	1.61	0.46
2:D:129:VAL:HB	2:D:229:LYS:HD3	1.97	0.46
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.77	0.46
1:C:108:ARG:HG2	1:C:108:ARG:NH1	2.30	0.46
1:A:186:TYR:CD1	1:A:192:TYR:CZ	3.04	0.46
2:F:153:LYS:HB2	2:F:153:LYS:HE3	1.67	0.46
2:F:206:THR:HA	2:F:211:GLN:OE1	2.16	0.46
1:A:48:ILE:HD13	1:A:64:GLY:N	2.30	0.46
1:A:61:ARG:NH2	1:A:82:ASP:OD1	2.49	0.46
2:F:134:PRO:O	2:F:136:CYS:N	2.49	0.46
1:A:11:LEU:HD21	1:A:19:VAL:HG11	1.97	0.45
2:D:230:LYS:O	2:D:232:GLU:HG3	2.16	0.45
1:A:111:ALA:O	1:A:139:PHE:HA	2.16	0.45
1:C:198:HIS:CE1	1:C:200:THR:HG23	2.51	0.45
2:B:170:ASN:O	2:B:172:GLY:N	2.49	0.45
1:C:149:LYS:HG2	1:C:154:GLU:HA	1.97	0.45
1:E:132:VAL:HG12	1:E:148:TRP:HH2	1.81	0.45
1:E:188:ARG:HG3	1:E:189:HIS:CD2	2.52	0.45
2:F:102:TYR:CD1	4:F:553:PNP:CM	2.99	0.45
1:A:133:VAL:HB	2:B:132:LEU:HD11	1.97	0.45
2:D:206:THR:HA	2:D:211:GLN:OE1	2.17	0.45
2:F:179:VAL:HA	2:F:199:VAL:HA	1.97	0.45
1:A:38:GLN:HG3	1:A:44:ILE:HG12	1.98	0.45
2:B:160:VAL:CG2	2:B:218:VAL:HG13	2.46	0.45
1:C:96:TYR:HD2	2:D:47:TRP:CE2	2.35	0.45
2:F:83:MET:HE3	2:F:94:TYR:CE2	2.51	0.45
1:C:189:HIS:O	1:C:211:ARG:HD3	2.17	0.45
2:D:220:HIS:HB3	2:D:225:THR:HB	1.97	0.45
1:E:58:VAL:HA	1:E:59:PRO:HD3	1.84	0.45
1:E:133:VAL:HG12	1:E:134:CYS:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:THR:O	2:F:85:SER:HB2	2.17	0.45
2:B:13:GLN:HA	2:B:118:SER:O	2.17	0.45
2:B:58:ILE:O	2:B:59:TYR:HD1	1.98	0.45
2:D:120:ALA:CB	2:D:156:PHE:CE1	3.00	0.45
2:D:181:THR:HG23	2:D:197:SER:HB2	1.99	0.45
2:F:102:TYR:CD1	4:F:553:PNP:HM3	2.52	0.45
1:A:164:THR:HG22	1:A:165:ASP:N	2.32	0.45
2:B:219:ALA:HB2	2:B:226:LYS:HG2	1.99	0.45
1:C:170:ASP:O	1:C:172:THR:HG23	2.17	0.45
1:C:186:TYR:HD1	1:C:192:TYR:OH	1.99	0.45
2:D:2:VAL:HG23	2:D:27:PHE:CD1	2.52	0.45
2:D:129:VAL:O	2:D:229:LYS:HE2	2.16	0.45
2:B:87:ARG:HD3	2:B:89:GLU:OE1	2.16	0.45
1:C:32:TYR:CE2	2:D:102:TYR:CZ	3.05	0.45
1:C:81:GLU:HG3	1:C:82:ASP:N	2.31	0.45
2:D:35:HIS:NE2	4:D:552:PNP:C2	2.80	0.45
2:F:6:GLU:CD	2:F:112:GLY:H	2.20	0.45
2:F:129:VAL:O	2:F:229:LYS:HE2	2.17	0.45
1:E:11:LEU:HD21	1:E:19:VAL:CG1	2.48	0.44
2:F:181:THR:HG23	2:F:197:SER:HB2	1.99	0.44
2:D:170:ASN:HD22	2:D:174:LEU:CB	2.30	0.44
1:A:136:LEU:HD23	1:A:144:ILE:HD11	1.99	0.44
2:D:234:ARG:NE	2:D:234:ARG:HA	2.32	0.44
1:C:118:PHE:CD1	1:C:118:PHE:N	2.85	0.44
2:D:102:TYR:CD1	4:D:552:PNP:CM	3.01	0.44
2:F:135:VAL:HG13	2:F:136:CYS:HG	1.77	0.44
1:A:190:ASN:OD1	1:A:210:ASN:ND2	2.51	0.44
2:B:34:MET:HB3	2:B:79:LEU:HD22	1.99	0.44
1:C:3:GLN:HA	1:C:3:GLN:NE2	2.32	0.44
1:C:48:ILE:HG22	1:C:49:TYR:N	2.33	0.44
1:E:182:THR:O	1:E:183:LYS:C	2.56	0.44
2:F:124:THR:HG21	2:F:222:ALA:O	2.17	0.44
1:A:46:ARG:NH1	2:B:107:ALA:HB2	2.33	0.44
2:B:91:THR:O	2:B:92:ALA:HB2	2.17	0.44
2:B:29:PHE:O	2:B:31:SER:N	2.51	0.44
2:B:130:TYR:HD2	2:B:151:LEU:HD23	1.82	0.44
2:D:64:VAL:HG11	2:D:68:PHE:CE2	2.53	0.44
2:D:87:ARG:HB3	2:D:89:GLU:OE2	2.18	0.44
2:D:160:VAL:CG2	2:D:218:VAL:HG13	2.48	0.44
2:B:142:THR:HG22	2:B:144:SER:OG	2.18	0.44
2:D:67:ARG:HD2	2:D:85:SER:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:THR:O	2:D:142:THR:CB	2.65	0.44
1:E:11:LEU:HD21	1:E:19:VAL:HG13	1.99	0.44
2:F:105:ARG:HH11	2:F:105:ARG:HG2	1.81	0.44
1:C:18:ARG:HG3	1:C:75:ILE:O	2.18	0.44
2:D:232:GLU:HA	2:D:233:PRO:HD3	1.90	0.44
1:E:49:TYR:O	1:E:50:ALA:HB3	2.17	0.44
1:E:164:THR:CG2	1:E:165:ASP:N	2.80	0.44
1:A:133:VAL:HG21	2:B:151:LEU:HD13	2.00	0.43
2:F:40:ALA:O	2:F:42:GLU:N	2.51	0.43
2:F:65:LYS:HE3	2:F:65:LYS:HB2	1.70	0.43
2:B:24:ALA:HB1	2:B:27:PHE:CE1	2.54	0.43
2:B:129:VAL:HA	2:B:151:LEU:O	2.18	0.43
2:B:134:PRO:C	2:B:136:CYS:N	2.72	0.43
2:D:29:PHE:CD2	2:D:77:ASN:HA	2.53	0.43
2:D:47:TRP:HH2	2:D:59:TYR:HB3	1.83	0.43
1:A:6:GLN:HB3	1:A:100:GLY:H	1.83	0.43
1:A:61:ARG:HH21	1:A:82:ASP:CG	2.22	0.43
2:B:54:GLY:O	2:B:55:SER:CB	2.66	0.43
2:D:34:MET:HB3	2:D:79:LEU:HD22	2.00	0.43
2:F:19:LYS:HE2	2:F:80:PHE:CD2	2.53	0.43
1:A:41:ASP:OD1	1:A:43:THR:HB	2.19	0.43
2:B:2:VAL:HA	2:B:25:SER:O	2.18	0.43
1:C:106:ILE:HB	1:C:166:GLN:NE2	2.34	0.43
1:A:3:GLN:HA	1:A:3:GLN:NE2	2.33	0.43
2:D:83:MET:HE3	2:D:94:TYR:CE2	2.53	0.43
1:C:119:PRO:HD3	2:D:136:CYS:SG	2.58	0.43
1:A:182:THR:O	1:A:183:LYS:C	2.57	0.43
1:A:186:TYR:HA	1:A:192:TYR:OH	2.19	0.43
2:B:100:ASP:O	2:B:104:SER:HB3	2.18	0.43
1:C:7:SER:HA	1:C:8:PRO:C	2.38	0.43
1:C:133:VAL:HB	2:D:132:LEU:CD1	2.49	0.43
2:D:153:LYS:HB2	2:D:153:LYS:HE3	1.74	0.43
1:E:198:HIS:CE1	1:E:200:THR:HG23	2.53	0.43
2:B:186:LEU:HD13	2:B:193:TYR:CZ	2.53	0.43
1:C:107:LEU:O	1:C:107:LEU:HG	2.18	0.43
1:E:133:VAL:CG1	1:E:134:CYS:N	2.82	0.43
1:A:2:ILE:HG23	1:A:27:GLN:HB2	2.01	0.43
2:B:84:THR:O	2:B:85:SER:HB2	2.18	0.43
2:D:100:ASP:O	2:D:104:SER:HB3	2.19	0.43
2:D:135:VAL:HB	2:D:235:GLY:OXT	2.19	0.43
1:E:36:LEU:HD11	2:F:109:TRP:CZ2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:ARG:HH22	1:E:111:ALA:HB2	1.83	0.43
2:B:38:ARG:HH11	2:B:46:GLU:CD	2.23	0.42
1:C:46:ARG:NH1	2:D:107:ALA:HB2	2.33	0.42
1:C:139:PHE:CE2	1:C:144:ILE:HB	2.53	0.42
2:D:127:PRO:CB	2:D:155:TYR:HB3	2.33	0.42
2:D:132:LEU:HB2	2:D:149:GLY:C	2.40	0.42
2:B:4:LEU:HA	2:B:23:ALA:O	2.19	0.42
2:B:98:ARG:NH2	2:B:106:GLY:C	2.73	0.42
2:B:156:PHE:CE1	2:B:157:PRO:HB3	2.53	0.42
2:D:84:THR:O	2:D:85:SER:HB2	2.19	0.42
1:E:149:LYS:HB2	1:E:193:THR:HB	2.01	0.42
1:A:34:SER:HB3	1:A:89:LEU:HB3	2.02	0.42
1:C:174:SER:HB3	2:D:182:PHE:HE2	1.84	0.42
2:D:135:VAL:CG1	2:D:136:CYS:SG	2.94	0.42
1:E:76:SER:O	1:E:77:SER:HB3	2.18	0.42
2:B:39:GLN:O	2:B:92:ALA:HB1	2.20	0.42
2:B:148:LEU:HD23	2:B:231:ILE:CG2	2.49	0.42
1:C:15:LEU:HD12	1:C:15:LEU:H	1.82	0.42
2:D:17:SER:OG	2:D:84:THR:HA	2.18	0.42
1:E:94:SER:O	1:E:96:TYR:N	2.52	0.42
1:A:10:SER:HA	1:A:103:LYS:H	1.84	0.42
1:A:132:VAL:HG12	1:A:148:TRP:CH2	2.51	0.42
2:F:91:THR:O	2:F:92:ALA:HB2	2.20	0.42
1:A:21:LEU:HD23	1:A:21:LEU:N	2.34	0.42
1:C:37:GLN:HG3	1:C:86:TYR:CE1	2.54	0.42
2:D:221:PRO:O	2:D:223:SER:N	2.52	0.42
2:B:6:GLU:CD	2:B:112:GLY:H	2.23	0.42
1:C:119:PRO:HB3	1:C:209:PHE:CE2	2.53	0.42
1:E:125:LEU:HD23	1:E:125:LEU:HA	1.85	0.42
1:A:107:LEU:HA	1:A:140:TYR:OH	2.19	0.42
2:B:121:LYS:HG3	2:B:124:THR:O	2.20	0.42
2:B:202:THR:O	2:B:203:SER:C	2.57	0.42
2:D:58:ILE:O	2:D:59:TYR:HD1	2.03	0.42
2:D:87:ARG:HG3	2:D:87:ARG:NH1	2.29	0.42
2:D:125:THR:HG22	2:D:126:ALA:N	2.35	0.42
2:F:37:VAL:HG21	2:F:109:TRP:CH2	2.54	0.42
2:F:105:ARG:CG	2:F:105:ARG:NH1	2.77	0.42
1:A:31:GLY:HA2	1:A:71:TYR:CE2	2.55	0.42
2:B:104:SER:O	2:B:105:ARG:CB	2.68	0.42
2:B:141:THR:O	2:B:142:THR:CB	2.68	0.42
2:F:186:LEU:HA	2:F:192:LEU:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:GLN:HG3	2:B:44:GLY:O	2.20	0.42
1:C:95:PRO:O	1:C:95:PRO:HG2	2.20	0.42
2:D:5:VAL:O	2:D:5:VAL:HG12	2.19	0.42
2:D:230:LYS:HD2	2:D:232:GLU:OE2	2.20	0.42
2:F:220:HIS:HB3	2:F:225:THR:HB	2.02	0.42
1:A:112:ALA:HB2	1:A:200:THR:OG1	2.20	0.41
1:C:48:ILE:HD13	1:C:64:GLY:N	2.35	0.41
1:C:119:PRO:HG3	1:C:209:PHE:CD2	2.55	0.41
2:F:10:GLY:HA3	2:F:18:ARG:HH21	1.80	0.41
2:F:82:GLN:HE21	2:F:83:MET:N	2.18	0.41
2:F:102:TYR:CE1	4:F:553:PNP:CM	3.03	0.41
1:A:189:HIS:O	1:A:211:ARG:HD3	2.21	0.41
2:B:11:LEU:HD11	2:B:156:PHE:HE1	1.84	0.41
2:D:146:VAL:O	2:D:146:VAL:HG13	2.20	0.41
1:A:203:SER:HA	1:A:204:PRO:HD3	1.92	0.41
2:B:14:PRO:HA	2:B:86:LEU:O	2.19	0.41
2:B:134:PRO:HG3	2:B:147:THR:O	2.19	0.41
1:E:7:SER:HA	1:E:8:PRO:C	2.41	0.41
2:F:230:LYS:O	2:F:232:GLU:N	2.53	0.41
2:B:155:TYR:CE1	2:B:193:TYR:CB	3.03	0.41
1:C:10:SER:HA	1:C:103:LYS:O	2.21	0.41
1:C:31:GLY:HA2	1:C:71:TYR:CE2	2.55	0.41
1:C:73:LEU:HD12	1:C:73:LEU:C	2.39	0.41
2:D:150:CYS:O	2:D:196:SER:HA	2.21	0.41
2:F:34:MET:HB3	2:F:79:LEU:HD22	2.02	0.41
2:B:87:ARG:HG3	2:B:87:ARG:NH1	2.27	0.41
1:C:116:SER:HB3	2:D:141:THR:HG23	2.03	0.41
2:D:67:ARG:O	2:D:84:THR:HB	2.20	0.41
1:E:24:ARG:NH1	1:E:69:SER:HB2	2.36	0.41
1:E:189:HIS:O	1:E:211:ARG:HD3	2.20	0.41
1:C:111:ALA:C	1:C:200:THR:HG21	2.41	0.41
2:D:65:LYS:HE3	2:D:65:LYS:HB2	1.85	0.41
1:C:22:THR:HG22	1:C:23:CYS:N	2.34	0.41
1:C:185:GLU:HG2	1:C:188:ARG:NE	2.24	0.41
1:A:46:ARG:NE	1:A:49:TYR:HB3	2.36	0.41
1:A:49:TYR:CE1	1:A:53:THR:HB	2.56	0.41
1:A:108:ARG:CD	1:A:170:ASP:O	2.67	0.41
1:A:193:THR:HG23	1:A:206:VAL:HG13	2.03	0.41
1:C:133:VAL:CB	2:D:132:LEU:HD11	2.50	0.41
2:D:91:THR:O	2:D:92:ALA:HB2	2.20	0.41
2:D:186:LEU:HD13	2:D:193:TYR:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:34:MET:HB2	2:F:79:LEU:HD13	2.03	0.41
2:F:219:ALA:HB2	2:F:226:LYS:HG2	2.02	0.41
1:A:51:ALA:O	1:A:52:SER:HB3	2.20	0.41
1:A:164:THR:HG22	1:A:165:ASP:O	2.21	0.41
1:A:206:VAL:HG12	1:A:207:LYS:N	2.35	0.41
1:C:120:PRO:HG2	1:C:186:TYR:CE2	2.56	0.40
1:C:164:THR:CG2	1:C:165:ASP:N	2.83	0.40
1:C:209:PHE:CG	1:C:210:ASN:N	2.87	0.40
2:D:61:ALA:HB3	2:D:64:VAL:HG22	2.02	0.40
1:E:176:SER:OG	2:F:182:PHE:CD2	2.71	0.40
1:E:190:ASN:HD21	1:E:210:ASN:HD21	1.70	0.40
2:F:131:PRO:HD3	2:F:229:LYS:HG2	2.03	0.40
1:A:174:SER:HB3	2:B:182:PHE:HE2	1.86	0.40
2:B:105:ARG:HH11	2:B:105:ARG:CG	2.34	0.40
1:C:34:SER:HB3	1:C:89:LEU:HB3	2.04	0.40
1:E:33:LEU:HD11	1:E:88:CYS:HB2	2.03	0.40
1:E:59:PRO:C	1:E:61:ARG:H	2.24	0.40
1:E:193:THR:OG1	1:E:208:SER:HB3	2.22	0.40
2:D:14:PRO:HA	2:D:86:LEU:O	2.21	0.40
2:D:157:PRO:O	2:D:220:HIS:NE2	2.54	0.40
2:D:170:ASN:HD22	2:D:174:LEU:HB2	1.86	0.40
1:E:149:LYS:HG2	1:E:154:GLU:HA	2.04	0.40
1:C:58:VAL:HA	1:C:59:PRO:HD3	1.85	0.40
2:D:233:PRO:O	2:D:234:ARG:CB	2.66	0.40
1:E:192:TYR:HB2	1:E:209:PHE:CE1	2.56	0.40
1:A:118:PHE:CE2	2:B:132:LEU:O	2.74	0.40
1:A:118:PHE:HE2	2:B:132:LEU:O	2.05	0.40
2:B:87:ARG:CG	2:B:87:ARG:NH1	2.84	0.40
2:B:134:PRO:O	2:B:135:VAL:HG12	2.22	0.40
1:C:47:LEU:HD23	1:C:62:PHE:CD2	2.57	0.40
2:D:83:MET:CE	2:D:94:TYR:CE2	3.05	0.40
2:D:102:TYR:CD1	4:D:552:PNP:HM3	2.57	0.40
2:D:104:SER:O	2:D:105:ARG:CB	2.68	0.40
1:E:18:ARG:HG3	1:E:76:SER:CA	2.45	0.40
1:E:107:LEU:HA	1:E:140:TYR:OH	2.21	0.40
1:E:190:ASN:CG	1:E:210:ASN:HD21	2.25	0.40
1:E:193:THR:CA	1:E:208:SER:HB3	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLN:N	1:C:185:GLU:OE2[1_544]	2.15	0.05

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	212/214 (99%)	182 (86%)	24 (11%)	6 (3%)	5 29
1	C	212/214 (99%)	176 (83%)	28 (13%)	8 (4%)	3 22
1	E	212/214 (99%)	183 (86%)	23 (11%)	6 (3%)	5 29
2	B	218/220 (99%)	175 (80%)	23 (11%)	20 (9%)	1 3
2	D	218/220 (99%)	175 (80%)	23 (11%)	20 (9%)	1 3
2	F	218/220 (99%)	175 (80%)	24 (11%)	19 (9%)	1 4
All	All	1290/1302 (99%)	1066 (83%)	145 (11%)	79 (6%)	1 12

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	41	PRO
2	B	57	THR
2	B	104	SER
2	B	120	ALA
2	B	121	LYS
2	B	135	VAL
2	B	136	CYS
2	B	234	ARG
1	C	94	SER
1	C	106	ILE
2	D	41	PRO
2	D	104	SER
2	D	120	ALA
2	D	136	CYS
2	D	138	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	234	ARG
1	E	94	SER
1	E	110	ASP
2	F	41	PRO
2	F	57	THR
2	F	104	SER
2	F	134	PRO
2	F	135	VAL
2	F	136	CYS
2	F	234	ARG
1	A	52	SER
1	A	110	ASP
2	B	30	SER
2	B	134	PRO
2	B	138	ASP
2	B	142	THR
2	B	171	SER
1	C	107	LEU
2	D	57	THR
2	D	134	PRO
2	D	135	VAL
2	D	141	THR
2	D	142	THR
2	D	222	ALA
2	F	120	ALA
2	F	124	THR
2	F	138	ASP
2	F	142	THR
2	F	222	ALA
1	A	213	GLU
2	B	7	SER
2	B	8	GLY
2	B	105	ARG
2	B	222	ALA
2	D	8	GLY
2	D	105	ARG
2	D	124	THR
1	E	60	LYS
2	F	119	ALA
2	F	141	THR
2	B	141	THR
2	B	173	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	52	SER
1	C	60	LYS
1	C	211	ARG
2	D	7	SER
2	D	173	SER
1	E	211	ARG
2	F	105	ARG
2	F	173	SER
1	A	94	SER
1	A	157	ASN
2	B	102	TYR
1	C	51	ALA
1	C	77	SER
1	E	51	ALA
1	E	52	SER
1	A	211	ARG
2	D	2	VAL
2	F	171	SER
2	D	231	ILE
2	D	221	PRO
2	F	231	ILE
2	F	8	GLY

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	190/190 (100%)	168 (88%)	22 (12%)	5 24
1	C	190/190 (100%)	168 (88%)	22 (12%)	5 24
1	E	190/190 (100%)	170 (90%)	20 (10%)	7 28
2	B	183/183 (100%)	155 (85%)	28 (15%)	2 13
2	D	183/183 (100%)	153 (84%)	30 (16%)	2 11
2	F	183/183 (100%)	152 (83%)	31 (17%)	2 10
All	All	1119/1119 (100%)	966 (86%)	153 (14%)	3 17

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	11	LEU
1	A	24	ARG
1	A	30	SER
1	A	33	LEU
1	A	55	ASP
1	A	61	ARG
1	A	83	PHE
1	A	105	GLU
1	A	108	ARG
1	A	116	SER
1	A	153	SER
1	A	154	GLU
1	A	155	ARG
1	A	160	LEU
1	A	169	LYS
1	A	177	SER
1	A	188	ARG
1	A	200	THR
1	A	208	SER
1	A	210	ASN
1	A	213	GLU
2	B	1	ASP
2	B	4	LEU
2	B	12	VAL
2	B	22	CYS
2	B	28	THR
2	B	30	SER
2	B	38	ARG
2	B	41	PRO
2	B	55	SER
2	B	56	SER
2	B	65	LYS
2	B	81	LEU
2	B	88	SER
2	B	121	LYS
2	B	136	CYS
2	B	138	ASP
2	B	159	PRO
2	B	164	THR
2	B	174	LEU
2	B	175	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	176	SER
2	B	179	VAL
2	B	195	LEU
2	B	206	THR
2	B	217	ASN
2	B	227	VAL
2	B	230	LYS
2	B	234	ARG
1	C	9	SER
1	C	11	LEU
1	C	24	ARG
1	C	30	SER
1	C	33	LEU
1	C	49	TYR
1	C	55	ASP
1	C	79	GLU
1	C	81	GLU
1	C	83	PHE
1	C	105	GLU
1	C	116	SER
1	C	118	PHE
1	C	153	SER
1	C	154	GLU
1	C	155	ARG
1	C	169	LYS
1	C	177	SER
1	C	188	ARG
1	C	201	SER
1	C	210	ASN
1	C	213	GLU
2	D	1	ASP
2	D	4	LEU
2	D	12	VAL
2	D	18	ARG
2	D	20	LEU
2	D	28	THR
2	D	30	SER
2	D	38	ARG
2	D	41	PRO
2	D	55	SER
2	D	56	SER
2	D	65	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	81	LEU
2	D	105	ARG
2	D	121	LYS
2	D	132	LEU
2	D	134	PRO
2	D	136	CYS
2	D	138	ASP
2	D	159	PRO
2	D	174	LEU
2	D	175	SER
2	D	176	SER
2	D	191	ASP
2	D	195	LEU
2	D	206	THR
2	D	217	ASN
2	D	227	VAL
2	D	230	LYS
2	D	234	ARG
1	E	5	THR
1	E	11	LEU
1	E	24	ARG
1	E	30	SER
1	E	33	LEU
1	E	49	TYR
1	E	55	ASP
1	E	80	SER
1	E	83	PHE
1	E	105	GLU
1	E	108	ARG
1	E	116	SER
1	E	153	SER
1	E	154	GLU
1	E	155	ARG
1	E	175	MET
1	E	177	SER
1	E	188	ARG
1	E	210	ASN
1	E	213	GLU
2	F	1	ASP
2	F	4	LEU
2	F	18	ARG
2	F	22	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	28	THR
2	F	30	SER
2	F	38	ARG
2	F	41	PRO
2	F	55	SER
2	F	56	SER
2	F	65	LYS
2	F	81	LEU
2	F	88	SER
2	F	105	ARG
2	F	121	LYS
2	F	134	PRO
2	F	136	CYS
2	F	138	ASP
2	F	159	PRO
2	F	164	THR
2	F	174	LEU
2	F	176	SER
2	F	179	VAL
2	F	191	ASP
2	F	195	LEU
2	F	203	SER
2	F	206	THR
2	F	217	ASN
2	F	227	VAL
2	F	230	LYS
2	F	234	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	137	ASN
1	A	145	ASN
1	A	190	ASN
1	A	210	ASN
1	A	212	ASN
2	B	170	ASN
2	B	187	GLN
1	C	3	GLN
1	C	37	GLN
1	C	137	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	145	ASN
1	C	210	ASN
2	D	82	GLN
2	D	170	ASN
2	D	187	GLN
1	E	3	GLN
1	E	137	ASN
1	E	210	ASN
2	F	82	GLN
2	F	170	ASN
2	F	187	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	PNP	F	553	-	13,14,14	4.37	6 (46%)	15,20,20	1.71	1 (6%)
4	PNP	D	552	-	13,14,14	2.49	4 (30%)	15,20,20	1.77	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PNP	B	551	-	13,14,14	3.16	5 (38%)	15,20,20	1.64	1 (6%)

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
4	PNP	F	553	-	-	0/6/9/9	0/1/1/1
4	PNP	D	552	-	-	0/6/9/9	0/1/1/1
4	PNP	B	551	-	-	0/6/9/9	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	553	PNP	P-O2P	-13.82	1.28	1.50
4	B	551	PNP	P-O2P	-8.56	1.36	1.50
4	D	552	PNP	P-O2P	-6.20	1.40	1.50
4	F	553	PNP	P-O3P	-4.61	1.45	1.54
4	B	551	PNP	P-O3P	-4.51	1.46	1.54
4	F	553	PNP	C3-C4	-3.71	1.31	1.38
4	B	551	PNP	P-CM	-3.65	1.67	1.77
4	D	552	PNP	P-O3P	-3.37	1.48	1.54
4	D	552	PNP	C3-C4	-2.97	1.33	1.38
4	D	552	PNP	O1P-C1	-2.95	1.33	1.40
4	F	553	PNP	O1P-C1	-2.77	1.34	1.40
4	F	553	PNP	C2-C1	-2.41	1.33	1.38
4	B	551	PNP	O1N-N	-2.14	1.19	1.22
4	B	551	PNP	C3-C4	-2.13	1.34	1.38
4	F	553	PNP	P-O1P	2.01	1.60	1.58

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	552	PNP	O1P-P-O2P	-6.25	98.18	112.79
4	F	553	PNP	O1P-P-O2P	-5.96	98.85	112.79
4	B	551	PNP	O1P-P-O2P	-5.70	99.46	112.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	553	PNP	3	0
4	D	552	PNP	4	0
4	B	551	PNP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.