Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 01:48 PM EDT

PDB ID	:	5C08
Title	:	1E6 TCR in Complex with HLA-A0e carrying RQWGPDPAAV
Authors	:	Rizkallah, P.J.; Bulek, A.M.; Cole, D.K.; Sewell, A.K.
Deposited on	:	2015-06-12
Resolution	:	2.33 Å(reported)

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

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

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

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

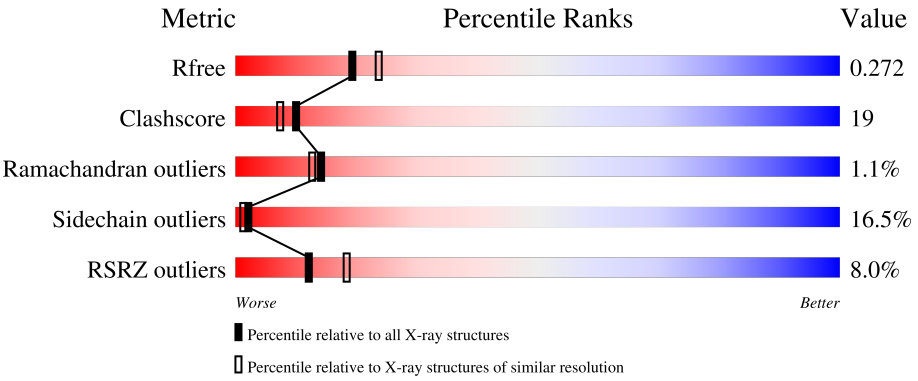
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.33 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.



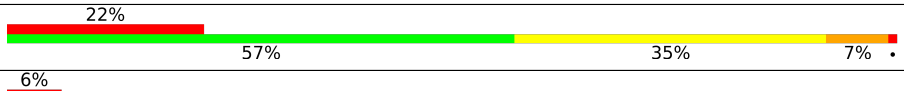
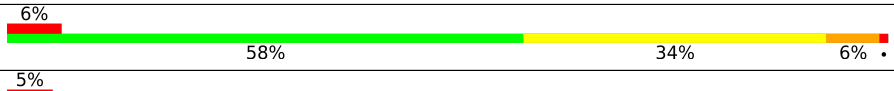
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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

Mol	Chain	Length	Quality of chain
1	A	276	4% 64% 26% 8%
1	F	276	3% 57% 32% 9%
2	B	100	% 62% 32% 5%
2	G	100	69% 25% 6%
3	C	10	80% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	10	
4	D	191	
4	I	191	
5	E	245	
5	J	245	

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
6	EDO	F	301	-	-	X	-
6	EDO	F	303	-	-	X	-
8	SO4	J	305	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 13627 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	F	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	G	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Marker peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			78	49	15	14			
3	H	10	Total	C	N	O	0	0	0
			78	49	15	14			

- Molecule 4 is a protein called 1E6 TCR Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	189	Total	C	N	O	S	0	0	0
			1488	927	248	303	10			

Continued on next page...

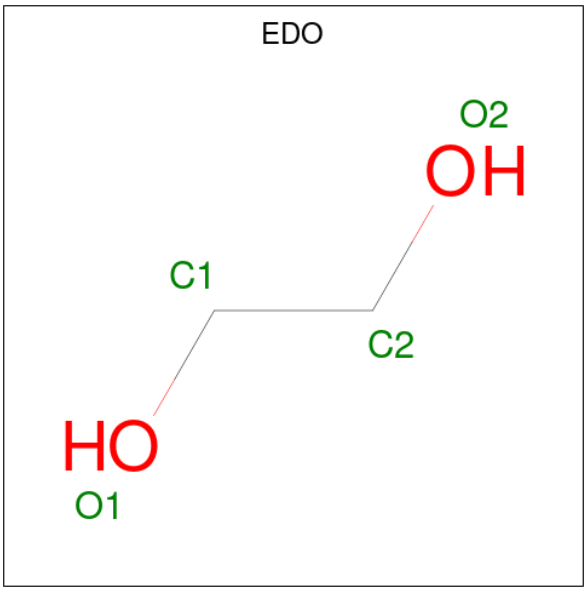
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	191	Total	C	N	O	S	0	0	0
			1501	936	250	305	10			

- Molecule 5 is a protein called 1E6 TCR Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	244	Total	C	N	O	S	0	0	0
			1961	1242	339	370	10			
5	J	245	Total	C	N	O	S	0	0	0
			1966	1245	340	371	10			

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



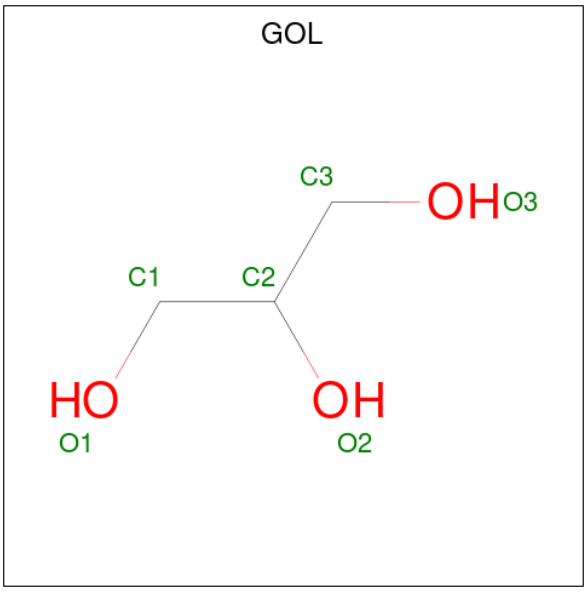
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

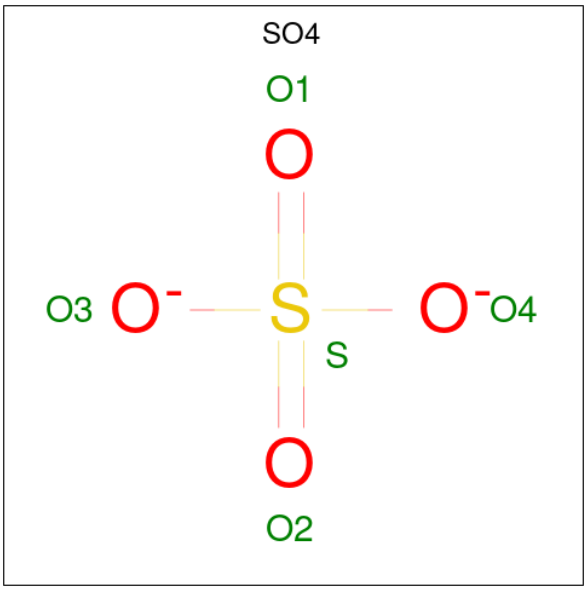
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	I	1	Total	C	O	0	0
			4	2	2		
6	I	1	Total	C	O	0	0
			4	2	2		
6	I	1	Total	C	O	0	0
			4	2	2		
6	I	1	Total	C	O	0	0
			4	2	2		
6	I	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total O S 5 4 1	0	0
8	E	1	Total O S 5 4 1	0	0
8	E	1	Total O S 5 4 1	0	0
8	F	1	Total O S 5 4 1	0	0
8	J	1	Total O S 5 4 1	0	0
8	J	1	Total O S 5 4 1	0	0

- Molecule 9 is water.

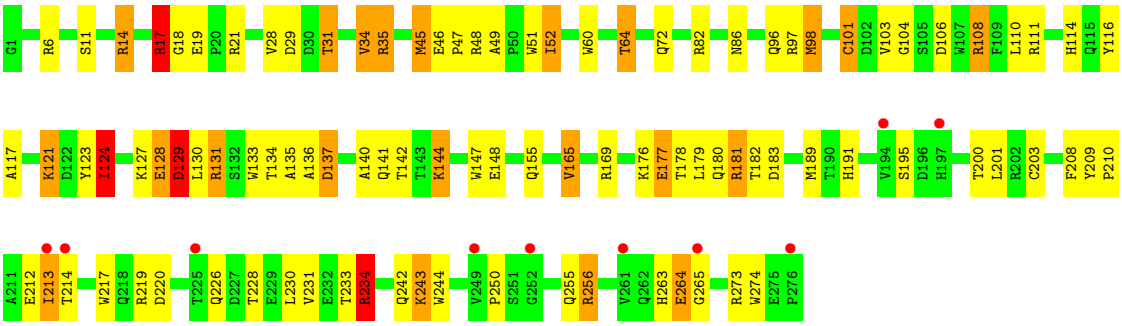
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	35	Total O 35 35	0	0
9	B	18	Total O 18 18	0	0
9	C	6	Total O 6 6	0	0
9	D	21	Total O 21 21	0	0
9	E	32	Total O 32 32	0	0
9	F	33	Total O 33 33	0	0
9	G	15	Total O 15 15	0	0
9	H	5	Total O 5 5	0	0
9	I	16	Total O 16 16	0	0
9	J	39	Total O 39 39	0	0

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.

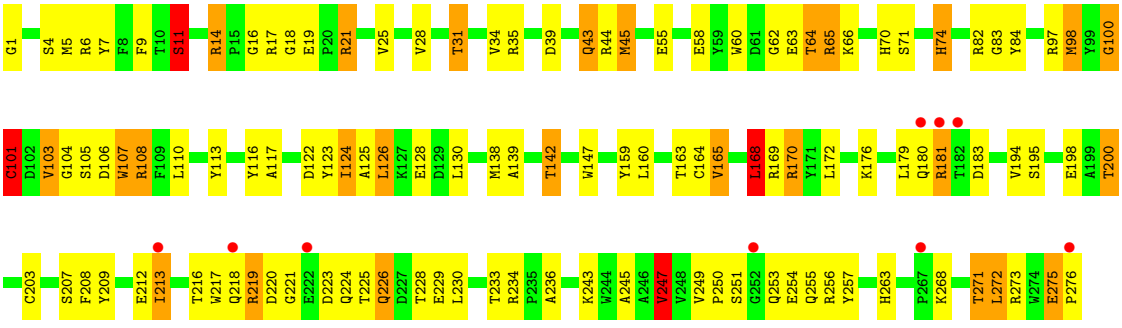
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A:



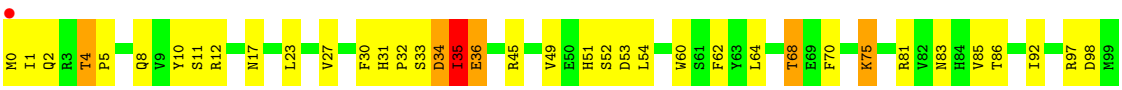
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain F:



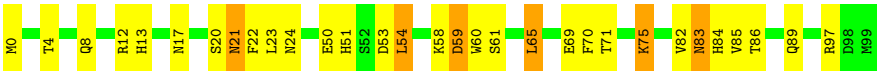
• Molecule 2: Beta-2-microglobulin

Chain B:



• Molecule 2: Beta-2-microglobulin

Chain G:

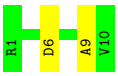


• Molecule 3: Marker peptide

Chain C:

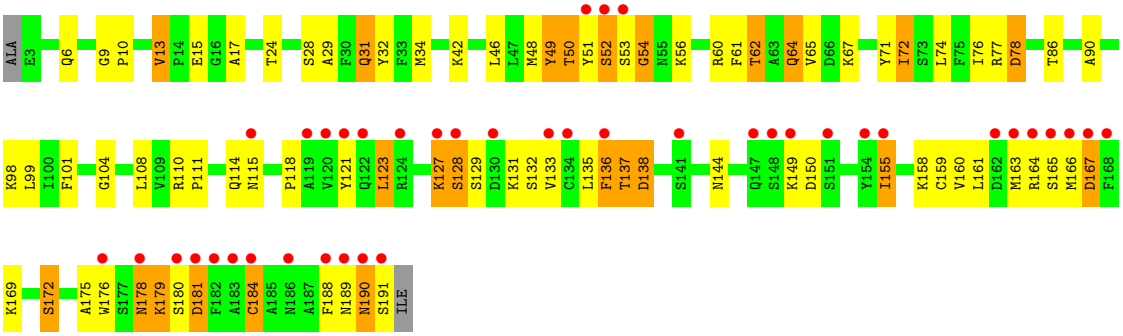
• Molecule 3: Marker peptide

Chain H:



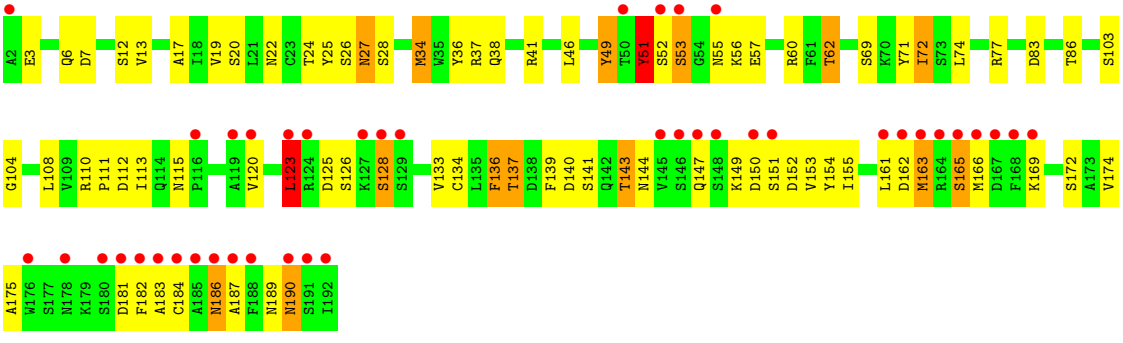
• Molecule 4: 1E6 TCR Alpha Chain

Chain D:



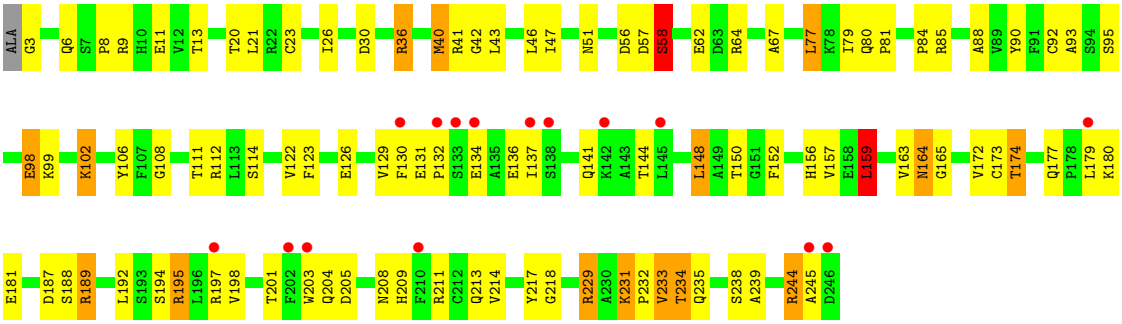
• Molecule 4: 1E6 TCR Alpha Chain

Chain I:



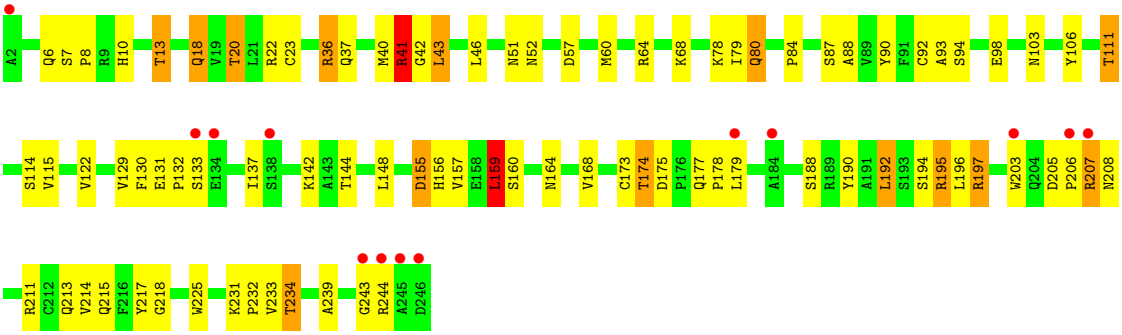
• Molecule 5: 1E6 TCR Beta Chain

Chain E:



• Molecule 5: 1E6 TCR Beta Chain

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	43.80Å 99.26Å 122.15Å 96.33° 98.07° 96.42°	Depositor
Resolution (Å)	48.91 – 2.33 48.91 – 2.33	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.91-2.33) 97.4 (48.91-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.206 , 0.272 0.206 , 0.272	Depositor DCC
R_{free} test set	4159 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13627	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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: EDO, SO4, 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	0.75	0/2320	0.98	9/3149 (0.3%)
1	F	0.76	0/2320	0.97	11/3149 (0.3%)
2	B	0.75	0/860	0.93	1/1162 (0.1%)
2	G	0.77	0/860	0.99	1/1162 (0.1%)
3	C	0.98	0/81	1.05	0/110
3	H	0.74	0/81	0.95	1/110 (0.9%)
4	D	0.74	0/1520	0.97	3/2055 (0.1%)
4	I	0.80	1/1533 (0.1%)	0.97	3/2073 (0.1%)
5	E	0.74	1/2016 (0.0%)	0.94	5/2741 (0.2%)
5	J	0.80	1/2021 (0.0%)	1.00	10/2748 (0.4%)
All	All	0.76	3/13612 (0.0%)	0.97	44/18459 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	F	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	94	SER	CB-OG	-8.10	1.31	1.42
4	I	36	TYR	CG-CD2	5.37	1.46	1.39
5	E	58	SER	CB-OG	-5.12	1.35	1.42

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	21	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	F	110	LEU	CA-CB-CG	8.20	134.17	115.30
1	A	230	LEU	CA-CB-CG	7.45	132.44	115.30
5	J	36	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	F	101	CYS	CB-CA-C	-7.32	95.76	110.40
1	A	234	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	F	21	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	17	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	A	110	LEU	CA-CB-CG	6.84	131.04	115.30
5	J	159	LEU	CA-CB-CG	6.77	130.88	115.30
1	F	168	LEU	CA-CB-CG	6.74	130.80	115.30
1	A	234	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	101	CYS	CA-CB-SG	-6.53	102.24	114.00
5	J	43	LEU	CA-CB-CG	6.44	130.11	115.30
5	J	197	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	F	39	ASP	CB-CG-OD1	6.35	124.02	118.30
5	E	57	ASP	N-CA-CB	-6.17	99.50	110.60
1	A	98	MET	CG-SD-CE	-6.15	90.36	100.20
4	D	78	ASP	CB-CG-OD2	-6.13	112.78	118.30
5	E	235	GLN	CB-CA-C	-6.05	98.30	110.40
2	B	35	ILE	CB-CA-C	-5.95	99.69	111.60
1	F	11	SER	CB-CA-C	5.93	121.37	110.10
4	D	78	ASP	CB-CG-OD1	5.73	123.46	118.30
4	I	34	MET	CG-SD-CE	-5.59	91.26	100.20
5	E	23	CYS	CA-CB-SG	-5.58	103.95	114.00
4	I	123	LEU	CA-CB-CG	5.53	128.01	115.30
2	G	54	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	129	ASP	CB-CG-OD2	5.47	123.22	118.30
1	F	247	VAL	CB-CA-C	-5.42	101.11	111.40
4	I	37	ARG	NE-CZ-NH2	-5.29	117.65	120.30
5	J	36	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	F	14	ARG	NE-CZ-NH2	-5.26	117.67	120.30
5	J	23	CYS	CA-CB-SG	-5.16	104.71	114.00
5	J	57	ASP	N-CA-CB	-5.16	101.31	110.60
1	F	21	ARG	CG-CD-NE	-5.15	100.99	111.80
5	J	179	LEU	CA-CB-CG	5.14	127.12	115.30
4	D	110	ARG	NE-CZ-NH2	5.09	122.84	120.30
5	J	41	ARG	NE-CZ-NH2	5.09	122.84	120.30
5	E	159	LEU	CA-CB-CG	5.08	126.98	115.30
5	J	51	ASN	CB-CA-C	-5.07	100.26	110.40
1	A	124	ILE	CB-CA-C	-5.05	101.50	111.60
1	F	65	ARG	NE-CZ-NH2	5.02	122.81	120.30
3	H	6	ASP	CB-CG-OD1	5.01	122.81	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	229	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Peptide
1	A	136	ALA	Peptide
1	F	100	GLY	Peptide

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	2254	0	2103	82	0
1	F	2254	0	2103	101	0
2	B	837	0	803	35	0
2	G	837	0	803	27	0
3	C	78	0	73	0	0
3	H	78	0	73	1	0
4	D	1488	0	1405	75	0
4	I	1501	0	1421	68	0
5	E	1961	0	1875	78	0
5	J	1966	0	1880	60	0
6	A	8	0	12	3	0
6	B	12	0	18	8	0
6	C	4	0	6	0	0
6	D	4	0	6	0	0
6	E	20	0	30	4	0
6	F	16	0	24	9	0
6	G	4	0	6	2	0
6	I	20	0	30	8	0
6	J	12	0	18	2	0
7	A	6	0	8	3	0
7	D	6	0	8	3	0
7	E	6	0	8	2	0
8	D	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	10	0	0	1	0
8	F	5	0	0	0	0
8	J	10	0	0	0	0
9	A	35	0	0	0	0
9	B	18	0	0	0	0
9	C	6	0	0	0	0
9	D	21	0	0	0	0
9	E	32	0	0	0	0
9	F	33	0	0	4	0
9	G	15	0	0	1	0
9	H	5	0	0	0	0
9	I	16	0	0	1	0
9	J	39	0	0	3	0
All	All	13627	0	12713	495	0

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

All (495) 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)
5:E:40:MET:CE	5:E:41:ARG:HH21	1.56	1.17
5:E:218:GLY:H	5:E:234:THR:HG22	1.04	1.16
5:E:40:MET:HE2	5:E:41:ARG:HH21	1.03	1.10
2:G:75:LYS:HE3	2:G:75:LYS:H	1.12	1.10
4:I:60:ARG:HD3	6:I:203:EDO:H21	1.14	1.06
2:G:4:THR:HG22	2:G:86:THR:OG1	1.56	1.04
1:F:213:ILE:CD1	1:F:243:LYS:HD2	1.89	1.03
4:I:62:THR:HG22	4:I:77:ARG:HH12	1.17	1.03
2:B:11:SER:O	6:B:301:EDO:H22	1.60	1.02
4:I:12:SER:H	6:I:201:EDO:H12	1.26	0.97
5:J:18:GLN:HB3	5:J:80:GLN:HG2	1.47	0.97
1:F:213:ILE:HD11	1:F:243:LYS:HD2	1.48	0.96
4:D:161:LEU:HD11	5:E:197:ARG:HH11	1.31	0.95
4:D:28:SER:O	4:D:29:ALA:HB3	1.64	0.94
4:D:133:VAL:HG12	4:D:176:TRP:HB3	1.48	0.93
5:J:18:GLN:CB	5:J:80:GLN:HG2	1.98	0.93
4:I:62:THR:CG2	4:I:77:ARG:HH12	1.82	0.92
1:A:128:GLU:O	1:A:129:ASP:HB3	1.69	0.91
1:A:106:ASP:OD1	1:A:108:ARG:HG3	1.71	0.91
5:E:40:MET:CE	5:E:41:ARG:NH2	2.34	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:TRP:O	1:A:64:THR:HG23	1.72	0.89
5:E:218:GLY:N	5:E:234:THR:HG22	1.87	0.88
1:F:6:ARG:HH11	6:F:301:EDO:H22	1.39	0.88
5:E:40:MET:HE2	5:E:41:ARG:NH2	1.88	0.87
1:F:18:GLY:O	1:F:19:GLU:HG3	1.73	0.87
4:I:137:THR:HG21	5:J:197:ARG:HH22	1.40	0.86
5:J:8:PRO:O	5:J:111:THR:HB	1.76	0.86
4:I:38:GLN:HE22	5:J:37:GLN:HE22	1.24	0.85
1:F:194:VAL:HB	1:F:200:THR:HG22	1.57	0.85
2:G:21:ASN:HD22	2:G:22:PHE:H	1.23	0.84
4:D:161:LEU:HD21	5:E:197:ARG:HH12	1.43	0.84
5:E:30:ASP:OD2	7:E:306:GOL:H31	1.77	0.83
5:J:164:ASN:HD21	5:J:208:ASN:HD22	1.23	0.83
4:I:51:TYR:HD1	4:I:51:TYR:H	1.23	0.83
4:D:161:LEU:HD11	5:E:197:ARG:NH1	1.93	0.82
5:J:157:VAL:HG13	5:J:214:VAL:HG13	1.61	0.81
4:I:123:LEU:HB3	5:J:131:GLU:O	1.81	0.81
4:D:28:SER:O	4:D:29:ALA:CB	2.28	0.81
4:D:132:SER:HA	5:E:130:PHE:HE2	1.44	0.80
2:G:75:LYS:HE3	2:G:75:LYS:N	1.95	0.80
2:B:53:ASP:HA	6:B:303:EDO:H21	1.62	0.80
5:J:36:ARG:NH2	6:J:303:EDO:O1	2.15	0.80
2:B:75:LYS:HE2	2:B:75:LYS:H	1.46	0.80
4:I:62:THR:HG22	4:I:77:ARG:NH1	1.97	0.79
5:J:41:ARG:HH21	5:J:41:ARG:HG2	1.47	0.79
4:D:121:TYR:HB2	4:D:135:LEU:HD21	1.65	0.79
1:F:106:ASP:HB3	1:F:108:ARG:H	1.48	0.79
1:A:14:ARG:HD3	1:A:19:GLU:O	1.82	0.79
2:G:4:THR:CG2	2:G:86:THR:OG1	2.30	0.79
5:E:41:ARG:HG3	5:E:42:GLY:O	1.82	0.78
1:F:60:TRP:O	1:F:64:THR:HG23	1.83	0.78
4:D:62:THR:HG22	4:D:77:ARG:HH22	1.49	0.78
1:A:96:GLN:HE22	2:B:31:HIS:HE1	1.28	0.77
1:F:6:ARG:HD2	6:F:301:EDO:H22	1.68	0.76
1:F:234:ARG:HH21	2:G:8:GLN:NE2	1.83	0.76
4:D:123:LEU:HB3	5:E:131:GLU:O	1.86	0.76
1:F:213:ILE:HD13	1:F:243:LYS:HD2	1.68	0.75
1:F:213:ILE:HD13	1:F:243:LYS:CD	2.16	0.75
4:I:57:GLU:HG2	4:I:62:THR:HB	1.68	0.75
1:A:35:ARG:HD3	1:A:48:ARG:NH1	2.02	0.75
4:D:62:THR:CG2	4:D:77:ARG:HH22	2.00	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:218:GLY:H	5:E:234:THR:CG2	1.94	0.73
4:I:183:ALA:O	4:I:184:CYS:HB2	1.89	0.73
5:E:41:ARG:HG3	5:E:42:GLY:N	2.03	0.73
1:F:106:ASP:HB3	1:F:108:ARG:HB3	1.69	0.73
1:F:55:GLU:OE2	1:F:170:ARG:NH1	2.23	0.72
1:F:213:ILE:CD1	1:F:243:LYS:CD	2.67	0.72
4:D:155:ILE:HG23	4:D:175:ALA:HB2	1.71	0.71
4:I:12:SER:N	6:I:201:EDO:H12	2.03	0.71
5:E:40:MET:HE1	5:E:41:ARG:HH21	1.55	0.71
4:D:121:TYR:HB2	4:D:135:LEU:CD2	2.21	0.70
5:E:30:ASP:OD2	7:E:306:GOL:C3	2.39	0.70
1:F:1:GLY:N	1:F:105:SER:HB3	2.07	0.70
1:F:219:ARG:HG2	1:F:224:GLN:HE21	1.57	0.69
5:J:164:ASN:HD21	5:J:208:ASN:ND2	1.89	0.69
5:E:40:MET:HE1	5:E:41:ARG:NH2	2.05	0.69
4:I:161:LEU:HB3	5:J:173:CYS:HB2	1.75	0.69
2:B:11:SER:O	6:B:301:EDO:C2	2.39	0.68
4:D:114:GLN:HE21	4:D:115:ASN:HD21	1.38	0.68
4:I:190:ASN:HD22	4:I:190:ASN:H	1.41	0.68
2:G:75:LYS:H	2:G:75:LYS:CE	2.00	0.68
2:G:13:HIS:H	2:G:21:ASN:HD21	1.42	0.67
4:I:151:SER:O	4:I:153:VAL:N	2.22	0.67
5:J:195:ARG:HD2	5:J:195:ARG:N	2.08	0.67
1:F:219:ARG:HB3	1:F:257:TYR:CE2	2.29	0.67
1:A:49:ALA:O	1:A:52:ILE:HD12	1.94	0.66
1:A:128:GLU:O	1:A:129:ASP:CB	2.43	0.66
4:D:65:VAL:HG13	4:D:72:ILE:HD11	1.78	0.66
4:I:52:SER:OG	4:I:53:SER:N	2.29	0.66
4:D:77:ARG:HH21	4:D:77:ARG:HG3	1.60	0.66
1:F:106:ASP:CB	1:F:108:ARG:HB3	2.25	0.66
4:D:6:GLN:NE2	4:D:104:GLY:H	1.95	0.65
5:J:18:GLN:HB2	5:J:80:GLN:HG2	1.77	0.65
4:I:147:GLN:HB3	4:I:155:ILE:CD1	2.27	0.65
2:B:45:ARG:HH12	6:B:302:EDO:C1	2.09	0.65
5:J:173:CYS:HB3	5:J:195:ARG:HD3	1.79	0.65
5:J:218:GLY:H	5:J:234:THR:HG22	1.62	0.64
4:D:114:GLN:HE21	4:D:115:ASN:ND2	1.95	0.64
2:G:17:ASN:HD21	2:G:97:ARG:HH22	1.46	0.64
1:F:213:ILE:HG23	1:F:263:HIS:HD2	1.62	0.64
1:A:116:TYR:HB3	1:A:124:ILE:HD12	1.80	0.64
4:D:52:SER:HB2	4:D:67:LYS:NZ	2.14	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:85:ARG:HB3	6:E:303:EDO:H22	1.80	0.63
1:F:228:THR:HG22	1:F:247:VAL:HG13	1.81	0.63
1:A:96:GLN:NE2	2:B:31:HIS:HE1	1.95	0.63
1:F:6:ARG:HD3	1:F:98:MET:HE3	1.81	0.63
1:A:35:ARG:HD3	1:A:48:ARG:CZ	2.29	0.62
1:A:97:ARG:HH11	1:A:114:HIS:CE1	2.17	0.62
1:F:125:ALA:HB2	6:F:303:EDO:H11	1.80	0.62
1:A:6:ARG:HD2	7:A:303:GOL:H31	1.81	0.62
1:A:182:THR:HG21	1:A:264:GLU:HG2	1.81	0.62
2:B:75:LYS:HE2	2:B:75:LYS:N	2.15	0.62
1:F:226:GLN:HA	1:F:226:GLN:NE2	2.13	0.62
1:A:34:VAL:HG22	1:A:45:MET:HE2	1.82	0.61
4:D:123:LEU:O	4:D:132:SER:HB2	1.99	0.61
1:A:195:SER:HA	1:F:229:GLU:OE1	2.00	0.61
2:G:21:ASN:ND2	2:G:22:PHE:H	1.94	0.61
1:A:35:ARG:O	1:A:45:MET:HE3	2.00	0.61
4:D:60:ARG:HE	7:D:202:GOL:H2	1.66	0.61
1:F:165:VAL:CG1	1:F:169:ARG:NH2	2.63	0.61
5:J:157:VAL:CG1	5:J:214:VAL:HG13	2.30	0.61
4:D:77:ARG:HG3	4:D:77:ARG:NH2	2.16	0.61
4:I:140:ASP:O	4:I:143:THR:HG22	2.00	0.61
5:J:41:ARG:HG2	5:J:41:ARG:NH2	2.16	0.61
4:D:132:SER:HA	5:E:130:PHE:CE2	2.32	0.61
5:J:36:ARG:HH22	6:J:303:EDO:C1	2.13	0.60
6:F:302:EDO:H21	3:H:9:ALA:HB2	1.83	0.60
4:I:19:VAL:HA	6:I:205:EDO:H21	1.84	0.60
5:E:204:GLN:HG2	5:E:245:ALA:HA	1.84	0.60
5:E:84:PRO:HB2	6:E:303:EDO:H11	1.84	0.60
2:B:4:THR:HG23	2:B:86:THR:OG1	2.02	0.59
1:F:1:GLY:H2	1:F:105:SER:HB3	1.66	0.59
4:I:137:THR:CG2	4:I:172:SER:HB3	2.33	0.59
4:I:120:VAL:HG22	4:I:136:PHE:HD2	1.67	0.59
2:B:45:ARG:HH22	6:B:302:EDO:H11	1.68	0.59
4:D:149:LYS:HG3	4:D:150:ASP:H	1.68	0.59
5:J:174:THR:HB	5:J:194:SER:HB2	1.84	0.59
4:D:123:LEU:HD11	4:D:135:LEU:HD22	1.85	0.59
1:F:62:GLY:O	1:F:66:LYS:HD2	2.02	0.59
1:A:29:ASP:O	7:A:303:GOL:H2	2.03	0.58
4:I:162:ASP:CB	4:I:169:LYS:HG2	2.33	0.58
5:J:133:SER:O	5:J:137:ILE:HG13	2.02	0.58
5:J:217:TYR:HA	5:J:234:THR:HB	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:HIS:CE1	1:F:97:ARG:HE	2.22	0.58
1:F:6:ARG:HD2	6:F:301:EDO:C2	2.32	0.58
5:J:84:PRO:HA	5:J:115:VAL:O	2.04	0.58
2:G:59:ASP:HB3	2:G:61:SER:H	1.68	0.58
1:A:220:ASP:OD2	1:A:256:ARG:HD2	2.03	0.58
4:D:13:VAL:HG13	4:D:17:ALA:HB3	1.86	0.58
1:F:6:ARG:NH1	6:F:301:EDO:H22	2.14	0.58
4:I:69:SER:HB3	6:I:204:EDO:H21	1.86	0.57
4:I:162:ASP:HB2	4:I:169:LYS:HG2	1.86	0.57
4:I:140:ASP:O	4:I:143:THR:CG2	2.53	0.57
1:F:65:ARG:NE	9:F:401:HOH:O	2.18	0.57
4:I:60:ARG:HD3	6:I:203:EDO:C2	2.09	0.57
1:F:195:SER:HB3	1:F:198:GLU:HB2	1.85	0.57
4:D:161:LEU:HD21	5:E:197:ARG:NH1	2.15	0.57
5:J:157:VAL:HA	5:J:215:GLN:O	2.05	0.57
1:A:97:ARG:HH11	1:A:114:HIS:HE1	1.52	0.56
2:B:45:ARG:HH12	6:B:302:EDO:H12	1.70	0.56
5:E:88:ALA:HB3	5:E:90:TYR:CE1	2.41	0.56
4:D:137:THR:HG22	4:D:172:SER:HB3	1.87	0.56
5:E:21:LEU:HD22	5:E:111:THR:HG21	1.88	0.56
1:F:124:ILE:HD13	1:F:147:TRP:CZ3	2.41	0.56
1:F:43:GLN:HG3	9:F:429:HOH:O	2.05	0.55
1:A:135:ALA:HB3	1:A:141:GLN:NE2	2.21	0.55
4:D:161:LEU:HB3	5:E:173:CYS:HB2	1.87	0.55
4:I:139:PHE:CD1	4:I:143:THR:CG2	2.90	0.55
1:A:263:HIS:CD2	1:A:265:GLY:H	2.25	0.55
5:E:56:ASP:OD1	5:E:58:SER:HB2	2.07	0.55
1:A:101:CYS:HB3	1:A:165:VAL:HG23	1.89	0.55
4:I:62:THR:CG2	4:I:77:ARG:NH1	2.60	0.55
5:J:157:VAL:HG13	5:J:214:VAL:CG1	2.32	0.55
1:F:253:GLN:CD	1:F:256:ARG:HH21	2.08	0.55
5:J:114:SER:OG	5:J:156:HIS:HE1	1.89	0.55
5:E:114:SER:HG	5:E:156:HIS:HE2	1.54	0.55
1:F:106:ASP:CB	1:F:108:ARG:H	2.16	0.55
1:F:213:ILE:HD13	1:F:243:LYS:HD3	1.86	0.55
4:I:147:GLN:HE21	4:I:149:LYS:CB	2.19	0.55
5:J:64:ARG:O	5:J:79:ILE:HA	2.06	0.55
1:F:168:LEU:O	1:F:172:LEU:HG	2.07	0.54
1:A:28:VAL:HG23	1:A:28:VAL:O	2.07	0.54
5:J:20:THR:HB	5:J:78:LYS:HG2	1.89	0.54
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:147:GLN:HE21	4:I:149:LYS:HB3	1.72	0.54
4:D:127:LYS:O	4:D:129:SER:N	2.41	0.54
1:F:103:VAL:HG13	1:F:107:TRP:HA	1.89	0.54
1:F:220:ASP:OD1	1:F:256:ARG:HD3	2.07	0.54
5:J:155:ASP:OD2	5:J:178:PRO:HG2	2.08	0.54
1:A:231:VAL:HG13	1:A:244:TRP:CH2	2.43	0.54
1:F:165:VAL:HG13	1:F:169:ARG:NH2	2.22	0.54
5:E:159:LEU:C	5:E:159:LEU:HD12	2.28	0.54
4:D:60:ARG:HG3	7:D:202:GOL:H31	1.88	0.54
5:E:211:ARG:NH2	6:E:301:EDO:O1	2.40	0.54
1:A:103:VAL:HG13	1:A:165:VAL:HG22	1.90	0.53
1:A:189:MET:HE1	1:A:274:TRP:HB2	1.91	0.53
1:A:213:ILE:HD13	1:A:243:LYS:HD2	1.89	0.53
1:F:230:LEU:HD23	1:F:245:ALA:HB2	1.89	0.53
1:F:11:SER:HB3	1:F:74:HIS:HD2	1.73	0.53
4:I:25:TYR:HE1	4:I:72:ILE:CD1	2.21	0.53
4:D:133:VAL:HG12	4:D:176:TRP:CB	2.30	0.53
4:I:60:ARG:CD	6:I:203:EDO:H21	2.09	0.53
1:F:183:ASP:O	1:F:208:PHE:HA	2.09	0.53
5:J:10:HIS:ND1	5:J:156:HIS:HD2	2.07	0.53
1:A:17:ARG:CD	1:A:18:GLY:H	2.22	0.53
1:F:250:PRO:HG2	1:F:253:GLN:NE2	2.24	0.53
4:D:190:ASN:O	4:D:191:SER:HB2	2.08	0.53
1:F:106:ASP:O	1:F:107:TRP:HB2	2.08	0.53
5:E:217:TYR:HA	5:E:234:THR:HB	1.91	0.52
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.43	0.52
1:A:17:ARG:HD2	1:A:18:GLY:H	1.75	0.52
5:E:231:LYS:HD2	5:E:233:VAL:HG23	1.91	0.52
4:I:162:ASP:O	4:I:163:MET:C	2.47	0.52
4:D:111:PRO:HG2	4:D:160:VAL:HG11	1.91	0.52
1:F:249:VAL:HG13	1:F:257:TYR:CE1	2.45	0.52
5:E:144:THR:HG21	5:E:197:ARG:NH2	2.24	0.52
1:A:104:GLY:HA3	1:A:108:ARG:NH1	2.25	0.52
4:D:51:TYR:C	4:D:53:SER:H	2.13	0.52
5:E:43:LEU:HD12	5:E:43:LEU:H	1.75	0.52
4:I:139:PHE:HD1	4:I:143:THR:CG2	2.22	0.52
1:A:31:THR:HG22	1:A:209:TYR:OH	2.10	0.52
1:A:31:THR:HG21	1:A:179:LEU:CD2	2.40	0.52
4:D:51:TYR:CG	4:D:51:TYR:O	2.63	0.52
1:A:177:GLU:O	1:A:181:ARG:HD3	2.10	0.51
4:I:139:PHE:CD1	4:I:143:THR:HG21	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:PRO:O	1:A:263:HIS:HE1	1.94	0.51
2:B:17:ASN:ND2	2:B:97:ARG:HH12	2.09	0.51
1:A:45:MET:HE3	1:A:45:MET:CA	2.40	0.51
1:A:189:MET:CE	1:A:201:LEU:HD22	2.41	0.51
1:A:45:MET:HE3	1:A:46:GLU:N	2.25	0.51
1:A:213:ILE:HD12	1:A:213:ILE:O	2.10	0.51
1:F:31:THR:HG22	1:F:209:TYR:CE2	2.46	0.51
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.46	0.51
1:F:14:ARG:HD2	1:F:21:ARG:H	1.76	0.51
4:I:72:ILE:HG23	9:I:512:HOH:O	2.11	0.51
4:D:62:THR:HG22	4:D:77:ARG:NH2	2.22	0.51
1:F:106:ASP:HB3	1:F:108:ARG:CB	2.37	0.51
1:F:213:ILE:HD12	1:F:213:ILE:O	2.10	0.51
4:D:161:LEU:HB3	5:E:173:CYS:CB	2.41	0.51
5:E:174:THR:HA	5:E:194:SER:HA	1.92	0.51
1:F:98:MET:HE1	1:F:113:TYR:HE1	1.76	0.51
2:G:53:ASP:HA	6:G:101:EDO:H11	1.93	0.51
1:A:35:ARG:N	1:A:45:MET:HE1	2.25	0.50
2:B:4:THR:HG22	2:B:5:PRO:HD2	1.92	0.50
1:A:234:ARG:HD2	1:A:242:GLN:OE1	2.11	0.50
2:B:31:HIS:CD2	2:B:32:PRO:HA	2.46	0.50
4:D:121:TYR:CE2	5:E:136:GLU:HB2	2.47	0.50
4:I:137:THR:HG22	4:I:172:SER:HB3	1.93	0.50
4:I:186:ASN:CG	4:I:187:ALA:H	2.15	0.50
5:E:6:GLN:NE2	5:E:92:CYS:H	2.09	0.50
1:F:203:CYS:HB2	1:F:217:TRP:CZ2	2.47	0.50
4:I:154:TYR:O	4:I:175:ALA:HA	2.11	0.50
1:A:45:MET:HB2	1:A:64:THR:HG22	1.94	0.50
4:I:181:ASP:N	4:I:181:ASP:OD1	2.45	0.50
4:D:62:THR:CG2	4:D:77:ARG:NH2	2.74	0.50
5:E:144:THR:HG21	5:E:197:ARG:HH21	1.75	0.50
1:F:28:VAL:HG23	1:F:179:LEU:HD21	1.94	0.50
1:A:127:LYS:HE2	1:A:134:THR:HG23	1.94	0.50
1:F:104:GLY:C	1:F:106:ASP:N	2.63	0.50
4:I:147:GLN:HB3	4:I:155:ILE:HD13	1.93	0.50
1:A:189:MET:CE	1:A:274:TRP:HB2	2.42	0.49
4:D:149:LYS:HG3	4:D:150:ASP:N	2.26	0.49
1:F:126:LEU:HD13	1:F:130:LEU:HA	1.92	0.49
1:A:34:VAL:HG22	1:A:45:MET:CE	2.42	0.49
1:A:123:TYR:CD2	1:A:124:ILE:HG13	2.47	0.49
1:A:231:VAL:HG13	1:A:244:TRP:CZ2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:179:LYS:H	4:D:179:LYS:HD2	1.76	0.49
1:F:70:HIS:HE1	1:F:74:HIS:CE1	2.30	0.49
1:F:218:GLN:O	1:F:257:TYR:HA	2.13	0.49
2:B:35:ILE:HD11	2:B:64:LEU:CD1	2.42	0.49
4:D:51:TYR:O	4:D:53:SER:N	2.45	0.49
4:D:137:THR:CG2	4:D:172:SER:HB3	2.43	0.49
5:E:122:VAL:HG12	5:E:232:PRO:HB2	1.95	0.49
2:G:83:ASN:HD22	2:G:84:HIS:H	1.61	0.49
4:I:139:PHE:HB2	4:I:143:THR:HG21	1.93	0.49
1:F:60:TRP:O	1:F:64:THR:CG2	2.57	0.49
4:I:24:THR:HG22	4:I:71:TYR:CD2	2.48	0.49
4:I:77:ARG:HG3	4:I:77:ARG:HH11	1.77	0.49
4:I:6:GLN:NE2	4:I:104:GLY:H	2.11	0.49
5:E:6:GLN:HE21	5:E:108:GLY:HA3	1.75	0.48
2:G:21:ASN:HD22	2:G:22:PHE:N	2.02	0.48
4:D:77:ARG:HH21	4:D:77:ARG:CG	2.26	0.48
1:A:11:SER:HA	1:A:21:ARG:O	2.13	0.48
1:A:133:TRP:HB2	1:A:144:LYS:HD3	1.95	0.48
5:E:129:VAL:HG23	5:E:239:ALA:HB3	1.94	0.48
5:E:8:PRO:HG3	5:E:11:GLU:HG2	1.94	0.48
5:J:174:THR:HB	5:J:194:SER:CB	2.43	0.48
1:A:49:ALA:O	1:A:52:ILE:CD1	2.60	0.48
1:F:138:MET:O	1:F:142:THR:HG22	2.14	0.48
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.49	0.48
4:D:172:SER:O	5:E:195:ARG:NH2	2.42	0.48
4:D:65:VAL:HG22	4:D:72:ILE:HG13	1.95	0.48
5:E:187:ASP:OD1	5:E:187:ASP:N	2.45	0.48
2:B:36:GLU:HG3	2:B:83:ASN:HB3	1.96	0.48
4:I:137:THR:HG23	4:I:172:SER:HB3	1.95	0.48
4:I:112:ASP:C	4:I:112:ASP:OD1	2.53	0.48
1:A:97:ARG:HD3	1:A:114:HIS:CE1	2.49	0.47
1:A:231:VAL:CG1	1:A:244:TRP:CZ2	2.97	0.47
1:F:65:ARG:CD	9:F:401:HOH:O	2.58	0.47
2:G:4:THR:HG23	2:G:86:THR:HB	1.96	0.47
4:I:27:ASN:HD22	4:I:28:SER:N	2.12	0.47
4:D:50:THR:HB	4:D:56:LYS:HG3	1.96	0.47
2:G:83:ASN:ND2	2:G:84:HIS:H	2.12	0.47
2:B:17:ASN:HD21	2:B:97:ARG:HH22	1.62	0.47
2:B:54:LEU:H	6:B:303:EDO:H12	1.78	0.47
1:F:103:VAL:CG1	1:F:107:TRP:HA	2.44	0.47
4:D:24:THR:HG22	4:D:71:TYR:CD1	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.50	0.47
4:D:34:MET:HE1	4:D:99:LEU:HD21	1.96	0.47
5:E:67:ALA:N	8:E:308:SO4:O1	2.24	0.47
5:J:175:ASP:HB2	5:J:192:LEU:CD2	2.44	0.47
5:E:85:ARG:H	6:E:303:EDO:H22	1.80	0.47
5:J:13:THR:CG2	9:J:432:HOH:O	2.63	0.47
2:B:51:HIS:HD2	2:B:52:SER:O	1.98	0.47
1:F:213:ILE:HG23	1:F:263:HIS:CD2	2.45	0.47
4:I:27:ASN:HD22	4:I:27:ASN:C	2.17	0.47
5:J:46:LEU:O	5:J:60:MET:HG2	2.15	0.47
2:B:49:VAL:HA	2:B:68:THR:HG23	1.96	0.47
1:F:14:ARG:NH1	1:F:19:GLU:O	2.34	0.47
6:A:302:EDO:H22	2:B:0:MET:HG3	1.96	0.46
1:A:35:ARG:HD3	1:A:48:ARG:HH11	1.80	0.46
4:D:136:PHE:O	4:D:172:SER:HA	2.15	0.46
4:D:176:TRP:CE3	5:E:148:LEU:HD11	2.50	0.46
5:E:132:PRO:HD2	5:E:203:TRP:CH2	2.49	0.46
1:F:122:ASP:HB3	6:F:303:EDO:H21	1.95	0.46
4:I:147:GLN:CB	4:I:155:ILE:HD13	2.44	0.46
1:A:17:ARG:HD2	1:A:18:GLY:N	2.30	0.46
5:J:122:VAL:HG12	5:J:232:PRO:HB2	1.98	0.46
2:B:81:ARG:HG3	2:B:92:ILE:HG12	1.97	0.46
4:D:31:GLN:HB2	4:D:32:TYR:CE1	2.51	0.46
4:D:77:ARG:O	4:D:78:ASP:C	2.54	0.46
5:E:131:GLU:OE2	5:E:244:ARG:NH2	2.49	0.46
2:B:75:LYS:H	2:B:75:LYS:CE	2.21	0.46
4:D:34:MET:HG3	4:D:49:TYR:HB2	1.97	0.46
1:F:220:ASP:OD1	1:F:256:ARG:CD	2.64	0.46
4:I:60:ARG:NH1	4:I:83:ASP:OD2	2.48	0.46
1:A:96:GLN:HE22	2:B:31:HIS:CE1	2.19	0.46
1:A:165:VAL:O	1:A:169:ARG:HG3	2.15	0.46
2:G:4:THR:CG2	2:G:86:THR:CB	2.94	0.46
4:D:48:MET:HE1	4:D:56:LYS:O	2.16	0.46
1:A:234:ARG:HH21	2:B:8:GLN:NE2	2.14	0.46
5:E:64:ARG:O	5:E:79:ILE:HA	2.16	0.46
1:F:28:VAL:CG2	1:F:179:LEU:HD21	2.46	0.46
1:F:63:GLU:OE1	1:F:66:LYS:NZ	2.42	0.46
5:J:159:LEU:HD22	5:J:214:VAL:HG22	1.97	0.46
5:J:205:ASP:OD1	5:J:207:ARG:HD3	2.15	0.46
5:J:225:TRP:CB	5:J:231:LYS:HG3	2.47	0.46
5:E:36:ARG:HD2	5:E:46:LEU:HD21	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:174:THR:HB	5:E:194:SER:HB2	1.97	0.45
1:F:176:LYS:O	1:F:180:GLN:HB2	2.16	0.45
4:D:48:MET:CE	4:D:56:LYS:O	2.65	0.45
4:D:137:THR:HB	4:D:138:ASP:OD1	2.16	0.45
5:E:172:VAL:HA	5:E:195:ARG:O	2.16	0.45
1:F:159:TYR:CE2	1:F:164:CYS:HB2	2.51	0.45
4:D:52:SER:HB2	4:D:67:LYS:HZ3	1.81	0.45
4:I:139:PHE:CD1	4:I:143:THR:HG23	2.51	0.45
1:F:219:ARG:HB3	1:F:257:TYR:CD2	2.52	0.45
1:F:271:THR:C	1:F:272:LEU:HD23	2.37	0.45
1:A:106:ASP:CG	1:A:108:ARG:HG3	2.36	0.45
5:E:179:LEU:HD12	5:E:180:LYS:H	1.82	0.45
2:G:12:ARG:NH1	9:G:201:HOH:O	2.49	0.45
4:I:133:VAL:HB	5:J:130:PHE:CD2	2.52	0.45
1:A:35:ARG:CD	1:A:48:ARG:NH1	2.78	0.45
5:E:80:GLN:HA	5:E:81:PRO:HA	1.73	0.45
5:E:137:ILE:O	5:E:141:GLN:HA	2.17	0.45
5:E:163:VAL:HA	5:E:209:HIS:O	2.16	0.45
5:E:211:ARG:NH1	5:E:213:GLN:OE1	2.50	0.45
1:A:183:ASP:O	1:A:208:PHE:HA	2.16	0.45
2:G:22:PHE:CE2	2:G:69:GLU:HG2	2.51	0.45
5:J:129:VAL:HG23	5:J:239:ALA:HB3	1.99	0.44
5:J:206:PRO:HA	5:J:243:GLY:O	2.15	0.44
5:E:80:GLN:HE21	5:E:80:GLN:HB3	1.55	0.44
1:F:1:GLY:H3	1:F:105:SER:HB3	1.80	0.44
1:F:98:MET:HE1	1:F:113:TYR:CE1	2.52	0.44
4:I:162:ASP:HB3	4:I:169:LYS:HG2	1.98	0.44
1:A:103:VAL:CG1	1:A:165:VAL:HG22	2.48	0.44
4:D:54:GLY:O	4:D:64:GLN:HA	2.18	0.44
5:E:93:ALA:HA	5:E:106:TYR:O	2.18	0.44
4:I:20:SER:H	6:I:205:EDO:C2	2.31	0.44
1:A:45:MET:HE3	1:A:45:MET:HA	1.99	0.44
1:A:121:LYS:NZ	6:A:302:EDO:H12	2.33	0.44
1:A:124:ILE:HD13	1:A:147:TRP:CZ3	2.53	0.44
4:D:51:TYR:C	4:D:53:SER:N	2.70	0.44
5:E:157:VAL:HG13	5:E:214:VAL:HG13	1.99	0.44
4:D:180:SER:O	4:D:181:ASP:CB	2.66	0.44
1:F:5:MET:HB2	1:F:168:LEU:HB3	2.00	0.44
1:F:139:ALA:O	1:F:142:THR:HG23	2.18	0.44
5:J:111:THR:CG2	9:J:426:HOH:O	2.66	0.44
1:A:28:VAL:HG21	1:A:179:LEU:CD1	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:142:LYS:HB3	5:J:197:ARG:HD3	1.99	0.44
1:A:144:LYS:O	1:A:148:GLU:HG3	2.18	0.44
2:B:35:ILE:HD11	2:B:64:LEU:HD12	1.99	0.44
2:G:24:ASN:HB3	2:G:65:LEU:HD21	2.00	0.44
5:J:155:ASP:HB3	5:J:190:TYR:CD2	2.52	0.44
5:J:156:HIS:HB3	5:J:217:TYR:HB2	1.98	0.44
1:F:45:MET:HB2	1:F:64:THR:HG22	2.00	0.43
1:F:122:ASP:HB3	6:F:303:EDO:C2	2.48	0.43
1:F:275:GLU:HA	1:F:276:PRO:HD2	1.80	0.43
4:I:134:CYS:O	4:I:174:VAL:HA	2.17	0.43
1:F:17:ARG:HG2	1:F:18:GLY:H	1.83	0.43
1:F:181:ARG:HA	1:F:181:ARG:HD3	1.64	0.43
1:F:7:TYR:HB3	1:F:9:PHE:CE1	2.53	0.43
6:A:302:EDO:C2	2:B:0:MET:HG3	2.48	0.43
1:F:100:GLY:O	1:F:160:LEU:HD22	2.18	0.43
1:F:194:VAL:CB	1:F:200:THR:HG22	2.40	0.43
1:A:45:MET:HE3	1:A:46:GLU:H	1.82	0.43
1:A:45:MET:H	1:A:64:THR:HB	1.83	0.43
1:A:176:LYS:O	1:A:180:GLN:HB2	2.19	0.43
1:F:45:MET:H	1:F:64:THR:HB	1.83	0.43
5:J:6:GLN:NE2	5:J:92:CYS:H	2.17	0.43
1:F:104:GLY:C	1:F:106:ASP:H	2.22	0.43
1:F:106:ASP:HB3	1:F:108:ARG:N	2.26	0.43
1:A:137:ASP:HB3	1:A:140:ALA:H	1.83	0.43
5:E:3:GLY:HA2	5:E:26:ILE:HG12	2.00	0.43
4:I:41:ARG:HH12	5:J:157:VAL:H	1.66	0.43
4:I:163:MET:O	4:I:166:MET:HB2	2.18	0.43
5:E:102:LYS:HE2	5:E:102:LYS:HB2	1.81	0.42
4:I:13:VAL:HG13	4:I:17:ALA:HB3	2.01	0.42
1:A:189:MET:HE1	1:A:201:LEU:HD22	1.99	0.42
5:E:43:LEU:HD12	5:E:43:LEU:N	2.33	0.42
5:E:99:LYS:HE3	5:E:106:TYR:OH	2.19	0.42
5:E:181:GLU:HB2	5:E:189:ARG:O	2.19	0.42
1:F:4:SER:HA	1:F:101:CYS:O	2.20	0.42
4:I:49:TYR:HD2	5:J:103:ASN:HD22	1.65	0.42
4:I:113:ILE:HD13	4:I:141:SER:OG	2.19	0.42
5:J:211:ARG:NH1	5:J:213:GLN:OE1	2.52	0.42
4:D:131:LYS:O	4:D:132:SER:HB3	2.19	0.42
1:F:123:TYR:CD2	1:F:124:ILE:HG13	2.54	0.42
1:A:96:GLN:NE2	2:B:31:HIS:CE1	2.82	0.42
4:D:9:GLY:HA3	4:D:10:PRO:HA	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:47:ILE:HA	5:E:56:ASP:O	2.19	0.42
5:E:123:PHE:CD1	5:E:189:ARG:HD2	2.55	0.42
5:E:46:LEU:HD13	5:E:77:LEU:HD11	2.01	0.42
1:F:194:VAL:HB	1:F:200:THR:CG2	2.40	0.42
1:F:219:ARG:C	1:F:221:GLY:H	2.21	0.42
2:B:34:ASP:OD1	2:B:34:ASP:N	2.37	0.42
5:J:225:TRP:CG	5:J:231:LYS:HG3	2.54	0.42
1:A:133:TRP:HB2	1:A:144:LYS:CD	2.48	0.42
2:B:27:VAL:HG23	2:B:30:PHE:CE1	2.55	0.42
1:F:16:GLY:N	9:F:402:HOH:O	2.42	0.42
1:F:126:LEU:CD1	1:F:130:LEU:HA	2.50	0.42
4:D:49:TYR:O	4:D:49:TYR:CG	2.73	0.42
1:F:124:ILE:C	6:F:303:EDO:H11	2.40	0.42
2:G:17:ASN:ND2	2:G:97:ARG:HH22	2.15	0.42
5:J:18:GLN:OE1	5:J:20:THR:HG22	2.20	0.42
2:G:17:ASN:ND2	2:G:97:ARG:HH12	2.18	0.41
1:A:28:VAL:HG21	1:A:179:LEU:HD11	2.02	0.41
1:A:72:GLN:HE21	5:E:51:ASN:HD22	1.68	0.41
4:D:90:ALA:HB2	4:D:101:PHE:CD2	2.55	0.41
5:E:98:GLU:H	5:E:98:GLU:HG3	1.20	0.41
5:E:163:VAL:C	5:E:165:GLY:N	2.74	0.41
4:D:123:LEU:N	4:D:123:LEU:HD12	2.35	0.41
1:F:83:GLY:O	1:F:84:TYR:C	2.58	0.41
1:F:224:GLN:NE2	1:F:257:TYR:HE2	2.18	0.41
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.56	0.41
4:D:123:LEU:HB2	5:E:130:PHE:HB3	2.03	0.41
2:G:4:THR:HG23	2:G:86:THR:CB	2.49	0.41
2:G:51:HIS:HA	2:G:65:LEU:O	2.20	0.41
4:D:61:PHE:CE2	4:D:76:ILE:HG12	2.55	0.41
5:E:152:PHE:CE1	5:E:157:VAL:HG21	2.56	0.41
5:J:42:GLY:HA3	9:J:415:HOH:O	2.20	0.41
5:J:87:SER:O	5:J:88:ALA:HB2	2.20	0.41
5:E:112:ARG:HG2	5:E:156:HIS:CE1	2.54	0.41
1:F:6:ARG:HB3	1:F:98:MET:HE3	2.02	0.41
4:I:51:TYR:CD1	4:I:51:TYR:N	2.76	0.41
5:J:36:ARG:HB2	5:J:46:LEU:HD11	2.02	0.41
4:D:164:ARG:O	4:D:165:SER:HB3	2.21	0.41
1:F:116:TYR:HB3	1:F:124:ILE:HD12	2.03	0.41
5:J:10:HIS:ND1	5:J:156:HIS:CD2	2.87	0.41
1:A:6:ARG:CD	7:A:303:GOL:H31	2.49	0.41
1:A:45:MET:HE2	1:A:45:MET:HB3	1.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:106:TYR:N	5:J:106:TYR:CD1	2.88	0.41
4:I:77:ARG:NH1	4:I:77:ARG:HG3	2.35	0.41
5:J:93:ALA:HA	5:J:106:TYR:O	2.20	0.41
5:J:132:PRO:HD2	5:J:203:TRP:CZ2	2.56	0.41
5:J:177:GLN:HA	5:J:178:PRO:HD3	1.90	0.41
1:A:47:PRO:HB3	1:A:52:ILE:HD13	2.03	0.41
5:E:194:SER:C	5:E:195:ARG:HD3	2.41	0.41
1:F:236:ALA:O	2:G:12:ARG:HD3	2.21	0.41
4:I:25:TYR:CE1	4:I:72:ILE:CD1	3.03	0.41
4:D:60:ARG:NE	7:D:202:GOL:H2	2.34	0.40
4:D:127:LYS:HE3	4:D:128:SER:H	1.86	0.40
4:I:110:ARG:HA	4:I:111:PRO:HD3	1.88	0.40
2:B:53:ASP:HA	6:B:303:EDO:C2	2.42	0.40
5:J:88:ALA:HB3	5:J:90:TYR:CE1	2.56	0.40
4:D:131:LYS:HE3	4:D:178:ASN:HA	2.04	0.40
4:D:136:PHE:CD1	4:D:136:PHE:N	2.89	0.40
2:G:53:ASP:HA	6:G:101:EDO:C1	2.51	0.40
2:B:27:VAL:HG23	2:B:30:PHE:HE1	1.86	0.40
4:D:169:LYS:HE3	4:D:169:LYS:HB3	1.91	0.40
5:E:164:ASN:HD21	5:E:208:ASN:HA	1.87	0.40
4:I:139:PHE:HD1	4:I:143:THR:HG23	1.86	0.40
4:I:147:GLN:HG3	4:I:189:ASN:ND2	2.37	0.40
1:F:165:VAL:HG13	1:F:169:ARG:CZ	2.52	0.40
4:I:125:ASP:OD1	4:I:126:SER:N	2.55	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	274/276 (99%)	267 (97%)	4 (2%)	3 (1%)	14 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	274/276 (99%)	265 (97%)	9 (3%)	0	100	100
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	G	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	H	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
4	D	187/191 (98%)	168 (90%)	12 (6%)	7 (4%)	3	1
4	I	189/191 (99%)	172 (91%)	11 (6%)	6 (3%)	4	1
5	E	242/245 (99%)	225 (93%)	15 (6%)	2 (1%)	19	20
5	J	243/245 (99%)	236 (97%)	7 (3%)	0	100	100
All	All	1621/1644 (99%)	1533 (95%)	70 (4%)	18 (1%)	14	13

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	128	SER
4	D	167	ASP
4	D	181	ASP
4	I	51	TYR
4	I	152	ASP
1	A	129	ASP
4	D	52	SER
4	D	54	GLY
4	D	184	CYS
5	E	40	MET
4	I	165	SER
4	D	118	PRO
4	I	128	SER
4	I	163	MET
4	I	186	ASN
1	A	264	GLU
5	E	164	ASN
1	A	250	PRO

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	232/232 (100%)	191 (82%)	41 (18%)	2 1
1	F	232/232 (100%)	186 (80%)	46 (20%)	1 1
2	B	95/95 (100%)	82 (86%)	13 (14%)	3 3
2	G	95/95 (100%)	79 (83%)	16 (17%)	2 1
3	C	7/7 (100%)	5 (71%)	2 (29%)	0 0
3	H	7/7 (100%)	7 (100%)	0	100 100
4	D	170/171 (99%)	137 (81%)	33 (19%)	1 1
4	I	171/171 (100%)	142 (83%)	29 (17%)	2 1
5	E	215/215 (100%)	185 (86%)	30 (14%)	3 3
5	J	215/215 (100%)	187 (87%)	28 (13%)	4 3
All	All	1439/1440 (100%)	1201 (84%)	238 (16%)	2 1

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	ARG
1	A	31	THR
1	A	34	VAL
1	A	35	ARG
1	A	45	MET
1	A	52	ILE
1	A	64	THR
1	A	82	ARG
1	A	86	ASN
1	A	98	MET
1	A	108	ARG
1	A	111	ARG
1	A	121	LYS
1	A	124	ILE
1	A	128	GLU
1	A	129	ASP
1	A	130	LEU
1	A	131	ARG
1	A	137	ASP
1	A	142	THR
1	A	144	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	155	GLN
1	A	165	VAL
1	A	177	GLU
1	A	178	THR
1	A	181	ARG
1	A	191	HIS
1	A	200	THR
1	A	212	GLU
1	A	213	ILE
1	A	214	THR
1	A	219	ARG
1	A	226	GLN
1	A	228	THR
1	A	233	THR
1	A	234	ARG
1	A	243	LYS
1	A	255	GLN
1	A	256	ARG
1	A	273	ARG
2	B	1	ILE
2	B	2	GLN
2	B	4	THR
2	B	12	ARG
2	B	23	LEU
2	B	34	ASP
2	B	35	ILE
2	B	36	GLU
2	B	68	THR
2	B	70	PHE
2	B	75	LYS
2	B	85	VAL
2	B	98	ASP
3	C	1	ARG
3	C	10	VAL
4	D	13	VAL
4	D	15	GLU
4	D	31	GLN
4	D	42	LYS
4	D	46	LEU
4	D	49	TYR
4	D	50	THR
4	D	62	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	64	GLN
4	D	72	ILE
4	D	74	LEU
4	D	86	THR
4	D	98	LYS
4	D	108	LEU
4	D	123	LEU
4	D	127	LYS
4	D	136	PHE
4	D	137	THR
4	D	138	ASP
4	D	144	ASN
4	D	155	ILE
4	D	158	LYS
4	D	159	CYS
4	D	163	MET
4	D	166	MET
4	D	167	ASP
4	D	172	SER
4	D	178	ASN
4	D	179	LYS
4	D	184	CYS
4	D	188	PHE
4	D	189	ASN
4	D	190	ASN
5	E	9	ARG
5	E	13	THR
5	E	20	THR
5	E	36	ARG
5	E	58	SER
5	E	62	GLU
5	E	77	LEU
5	E	95	SER
5	E	98	GLU
5	E	102	LYS
5	E	126	GLU
5	E	134	GLU
5	E	148	LEU
5	E	150	THR
5	E	159	LEU
5	E	174	THR
5	E	177	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	188	SER
5	E	189	ARG
5	E	192	LEU
5	E	195	ARG
5	E	198	VAL
5	E	201	THR
5	E	205	ASP
5	E	229	ARG
5	E	231	LYS
5	E	233	VAL
5	E	234	THR
5	E	238	SER
5	E	244	ARG
1	F	11	SER
1	F	25	VAL
1	F	31	THR
1	F	34	VAL
1	F	35	ARG
1	F	43	GLN
1	F	44	ARG
1	F	45	MET
1	F	58	GLU
1	F	64	THR
1	F	71	SER
1	F	74	HIS
1	F	82	ARG
1	F	98	MET
1	F	101	CYS
1	F	103	VAL
1	F	107	TRP
1	F	108	ARG
1	F	124	ILE
1	F	126	LEU
1	F	128	GLU
1	F	142	THR
1	F	163	THR
1	F	165	VAL
1	F	168	LEU
1	F	170	ARG
1	F	181	ARG
1	F	200	THR
1	F	207	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	212	GLU
1	F	213	ILE
1	F	216	THR
1	F	219	ARG
1	F	223	ASP
1	F	225	THR
1	F	226	GLN
1	F	233	THR
1	F	247	VAL
1	F	251	SER
1	F	254	GLU
1	F	255	GLN
1	F	268	LYS
1	F	271	THR
1	F	272	LEU
1	F	273	ARG
1	F	275	GLU
2	G	0	MET
2	G	20	SER
2	G	21	ASN
2	G	23	LEU
2	G	50	GLU
2	G	54	LEU
2	G	58	LYS
2	G	59	ASP
2	G	65	LEU
2	G	70	PHE
2	G	71	THR
2	G	75	LYS
2	G	82	VAL
2	G	83	ASN
2	G	85	VAL
2	G	89	GLN
4	I	3	GLU
4	I	7	ASP
4	I	22	ASN
4	I	26	SER
4	I	27	ASN
4	I	34	MET
4	I	46	LEU
4	I	49	TYR
4	I	51	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	I	53	SER
4	I	55	ASN
4	I	56	LYS
4	I	62	THR
4	I	72	ILE
4	I	74	LEU
4	I	86	THR
4	I	103	SER
4	I	108	LEU
4	I	115	ASN
4	I	123	LEU
4	I	128	SER
4	I	136	PHE
4	I	137	THR
4	I	143	THR
4	I	144	ASN
4	I	150	ASP
4	I	165	SER
4	I	182	PHE
4	I	190	ASN
5	J	7	SER
5	J	13	THR
5	J	18	GLN
5	J	20	THR
5	J	22	ARG
5	J	40	MET
5	J	41	ARG
5	J	43	LEU
5	J	52	ASN
5	J	68	LYS
5	J	80	GLN
5	J	98	GLU
5	J	111	THR
5	J	144	THR
5	J	148	LEU
5	J	155	ASP
5	J	159	LEU
5	J	160	SER
5	J	168	VAL
5	J	174	THR
5	J	188	SER
5	J	192	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	J	195	ARG
5	J	196	LEU
5	J	207	ARG
5	J	233	VAL
5	J	234	THR
5	J	244	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	96	GLN
1	A	114	HIS
1	A	141	GLN
1	A	151	HIS
1	A	174	ASN
1	A	180	GLN
1	A	191	HIS
1	A	263	HIS
2	B	2	GLN
2	B	8	GLN
2	B	17	ASN
2	B	31	HIS
2	B	51	HIS
4	D	6	GLN
4	D	38	GLN
4	D	115	ASN
4	D	190	ASN
5	E	6	GLN
5	E	37	GLN
5	E	51	ASN
5	E	80	GLN
5	E	121	ASN
5	E	164	ASN
5	E	209	HIS
1	F	43	GLN
1	F	70	HIS
1	F	72	GLN
1	F	74	HIS
1	F	86	ASN
1	F	151	HIS
1	F	180	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	191	HIS
1	F	224	GLN
1	F	226	GLN
1	F	253	GLN
2	G	8	GLN
2	G	17	ASN
2	G	21	ASN
2	G	83	ASN
4	I	6	GLN
4	I	27	ASN
4	I	142	GLN
4	I	147	GLN
4	I	190	ASN
5	J	6	GLN
5	J	37	GLN
5	J	51	ASN
5	J	139	HIS
5	J	156	HIS
5	J	208	ASN
5	J	235	GLN

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

35 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	$\#\|Z\| > 2$
6	EDO	E	305	-	3,3,3	0.72	0	2,2,2	0.08	0
6	EDO	G	101	-	3,3,3	0.52	0	2,2,2	0.28	0
6	EDO	B	301	-	3,3,3	0.34	0	2,2,2	0.43	0
6	EDO	J	301	-	3,3,3	0.49	0	2,2,2	0.31	0
6	EDO	J	302	-	3,3,3	0.53	0	2,2,2	0.64	0
8	SO4	J	304	-	4,4,4	0.49	0	6,6,6	0.34	0
6	EDO	I	205	-	3,3,3	0.71	0	2,2,2	0.39	0
6	EDO	A	301	-	3,3,3	0.56	0	2,2,2	0.63	0
6	EDO	J	303	-	3,3,3	0.71	0	2,2,2	0.54	0
6	EDO	C	101	-	3,3,3	0.52	0	2,2,2	0.37	0
8	SO4	E	308	-	4,4,4	0.38	0	6,6,6	0.42	0
6	EDO	F	303	-	3,3,3	0.73	0	2,2,2	0.73	0
6	EDO	B	303	-	3,3,3	0.39	0	2,2,2	0.54	0
6	EDO	E	304	-	3,3,3	0.64	0	2,2,2	0.73	0
7	GOL	A	303	-	5,5,5	0.78	0	5,5,5	1.33	0
6	EDO	I	204	-	3,3,3	0.59	0	2,2,2	0.23	0
6	EDO	D	201	-	3,3,3	0.42	0	2,2,2	1.01	0
6	EDO	A	302	-	3,3,3	0.52	0	2,2,2	0.39	0
6	EDO	I	201	-	3,3,3	0.42	0	2,2,2	0.73	0
7	GOL	E	306	-	5,5,5	0.47	0	5,5,5	0.66	0
6	EDO	E	303	-	3,3,3	0.44	0	2,2,2	0.51	0
6	EDO	F	304	-	3,3,3	0.68	0	2,2,2	0.15	0
8	SO4	F	305	-	4,4,4	0.46	0	6,6,6	0.28	0
8	SO4	J	305	-	4,4,4	0.57	0	6,6,6	0.28	0
6	EDO	E	302	-	3,3,3	0.44	0	2,2,2	0.46	0
8	SO4	D	203	-	4,4,4	0.43	0	6,6,6	0.13	0
7	GOL	D	202	-	5,5,5	0.42	0	5,5,5	0.56	0
8	SO4	D	204	-	4,4,4	0.52	0	6,6,6	0.57	0
6	EDO	F	302	-	3,3,3	0.52	0	2,2,2	0.62	0
6	EDO	B	302	-	3,3,3	0.63	0	2,2,2	0.16	0
6	EDO	I	203	-	3,3,3	0.74	0	2,2,2	0.32	0
6	EDO	F	301	-	3,3,3	0.72	0	2,2,2	0.49	0
6	EDO	I	202	-	3,3,3	0.64	0	2,2,2	0.22	0
6	EDO	E	301	-	3,3,3	0.61	0	2,2,2	0.23	0
8	SO4	E	307	-	4,4,4	0.48	0	6,6,6	0.40	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
6	EDO	E	305	-	-	1/1/1/1	-
6	EDO	G	101	-	-	1/1/1/1	-
6	EDO	B	301	-	-	1/1/1/1	-
6	EDO	J	301	-	-	1/1/1/1	-
6	EDO	J	302	-	-	0/1/1/1	-
6	EDO	I	205	-	-	1/1/1/1	-
6	EDO	A	301	-	-	1/1/1/1	-
6	EDO	J	303	-	-	1/1/1/1	-
6	EDO	C	101	-	-	0/1/1/1	-
6	EDO	F	303	-	-	1/1/1/1	-
6	EDO	B	303	-	-	0/1/1/1	-
6	EDO	E	304	-	-	1/1/1/1	-
7	GOL	A	303	-	-	0/4/4/4	-
6	EDO	I	204	-	-	1/1/1/1	-
6	EDO	D	201	-	-	0/1/1/1	-
6	EDO	A	302	-	-	0/1/1/1	-
6	EDO	I	201	-	-	0/1/1/1	-
7	GOL	E	306	-	-	2/4/4/4	-
6	EDO	E	303	-	-	1/1/1/1	-
6	EDO	F	304	-	-	1/1/1/1	-
6	EDO	E	302	-	-	1/1/1/1	-
7	GOL	D	202	-	-	1/4/4/4	-
6	EDO	F	302	-	-	1/1/1/1	-
6	EDO	B	302	-	-	1/1/1/1	-
6	EDO	I	203	-	-	0/1/1/1	-
6	EDO	F	301	-	-	1/1/1/1	-
6	EDO	I	202	-	-	0/1/1/1	-
6	EDO	E	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	301	EDO	O1-C1-C2-O2
7	E	306	GOL	C1-C2-C3-O3
6	F	302	EDO	O1-C1-C2-O2
7	E	306	GOL	O2-C2-C3-O3
6	E	304	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	E	305	EDO	O1-C1-C2-O2
6	F	301	EDO	O1-C1-C2-O2
6	F	303	EDO	O1-C1-C2-O2
6	J	301	EDO	O1-C1-C2-O2
6	J	303	EDO	O1-C1-C2-O2
6	E	302	EDO	O1-C1-C2-O2
6	G	101	EDO	O1-C1-C2-O2
6	I	205	EDO	O1-C1-C2-O2
6	B	302	EDO	O1-C1-C2-O2
6	E	301	EDO	O1-C1-C2-O2
6	F	304	EDO	O1-C1-C2-O2
6	E	303	EDO	O1-C1-C2-O2
6	A	301	EDO	O1-C1-C2-O2
6	I	204	EDO	O1-C1-C2-O2
7	D	202	GOL	O2-C2-C3-O3

There are no ring outliers.

19 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	101	EDO	2	0
6	B	301	EDO	2	0
6	I	205	EDO	2	0
6	J	303	EDO	2	0
8	E	308	SO4	1	0
6	F	303	EDO	4	0
6	B	303	EDO	3	0
7	A	303	GOL	3	0
6	I	204	EDO	1	0
6	A	302	EDO	3	0
6	I	201	EDO	2	0
7	E	306	GOL	2	0
6	E	303	EDO	3	0
7	D	202	GOL	3	0
6	F	302	EDO	1	0
6	B	302	EDO	3	0
6	I	203	EDO	3	0
6	F	301	EDO	4	0
6	E	301	EDO	1	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

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	276/276 (100%)	0.36	10 (3%) 42 53	24, 48, 97, 125	0
1	F	276/276 (100%)	0.34	9 (3%) 46 57	24, 52, 88, 101	0
2	B	100/100 (100%)	-0.02	1 (1%) 82 88	31, 46, 65, 98	0
2	G	100/100 (100%)	0.04	0 100 100	32, 45, 66, 74	0
3	C	10/10 (100%)	0.18	0 100 100	27, 29, 33, 45	0
3	H	10/10 (100%)	0.06	0 100 100	29, 32, 33, 44	0
4	D	189/191 (98%)	1.09	41 (21%) 0 1	29, 55, 124, 140	0
4	I	191/191 (100%)	0.98	42 (21%) 0 1	28, 55, 119, 141	0
5	E	244/245 (99%)	0.46	15 (6%) 21 30	21, 52, 107, 128	0
5	J	245/245 (100%)	0.28	13 (5%) 26 37	22, 46, 85, 111	0
All	All	1641/1644 (99%)	0.47	131 (7%) 12 18	21, 49, 105, 141	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	191	SER	12.0
4	D	190	ASN	11.2
4	I	191	SER	8.8
5	E	138	SER	8.1
4	I	128	SER	7.8
4	D	128	SER	7.6
4	D	182	PHE	7.0
5	E	245	ALA	6.8
4	I	192	ILE	6.6
4	I	148	SER	6.4
4	D	149	LYS	6.4
4	I	166	MET	6.4
4	I	167	ASP	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	I	165	SER	5.9
4	D	151	SER	5.6
4	I	168	PHE	5.5
5	E	133	SER	5.3
5	E	246	ASP	5.1
5	J	245	ALA	5.0
4	D	166	MET	5.0
4	I	145	VAL	4.9
4	I	2	ALA	4.9
4	D	119	ALA	4.9
1	A	197	HIS	4.8
5	E	134	GLU	4.8
5	E	137	ILE	4.6
4	D	164	ARG	4.6
4	D	121	TYR	4.6
4	I	180	SER	4.5
5	J	246	ASP	4.4
4	D	165	SER	4.4
4	D	188	PHE	4.3
4	I	164	ARG	4.3
4	D	183	ALA	4.2
4	D	168	PHE	4.1
4	D	52	SER	4.0
4	I	187	ALA	3.9
1	F	181	ARG	3.9
4	I	182	PHE	3.9
4	D	180	SER	3.8
1	F	276	PRO	3.8
2	B	0	MET	3.8
1	A	276	PRO	3.7
1	A	265	GLY	3.7
4	I	161	LEU	3.6
4	I	52	SER	3.6
5	J	244	ARG	3.5
4	D	167	ASP	3.5
4	D	53	SER	3.5
4	D	186	ASN	3.4
4	D	51	TYR	3.4
5	E	202	PHE	3.3
5	J	243	GLY	3.3
4	D	124	ARG	3.3
1	A	194	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	189	ASN	3.2
4	D	147	GLN	3.2
5	J	134	GLU	3.2
4	D	155	ILE	3.2
1	A	249	VAL	3.1
5	E	210	PHE	3.1
4	D	122	GLN	3.1
4	I	147	GLN	3.1
5	E	203	TRP	3.1
4	I	150	ASP	3.1
4	I	162	ASP	3.0
1	A	252	GLY	3.0
4	D	133	VAL	3.0
5	E	197	ARG	3.0
4	I	129	SER	2.9
5	E	179	LEU	2.9
4	D	163	MET	2.9
5	E	145	LEU	2.8
4	I	178	ASN	2.8
4	I	53	SER	2.8
4	I	188	PHE	2.8
4	D	148	SER	2.8
4	D	181	ASP	2.7
4	I	184	CYS	2.7
4	I	169	LYS	2.7
1	F	180	GLN	2.7
4	D	120	VAL	2.7
5	E	132	PRO	2.7
5	E	142	LYS	2.7
4	I	181	ASP	2.7
4	I	50	THR	2.6
1	F	252	GLY	2.6
4	D	176	TRP	2.6
4	D	134	CYS	2.6
4	I	116	PRO	2.6
1	F	218	GLN	2.6
5	E	130	PHE	2.5
1	F	182	THR	2.5
4	I	55	ASN	2.5
4	I	186	ASN	2.5
4	I	146	SER	2.4
5	J	138	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	J	179	LEU	2.4
4	I	183	ALA	2.4
4	I	163	MET	2.4
4	D	154	TYR	2.4
4	I	185	ALA	2.4
4	D	141	SER	2.3
4	D	115	ASN	2.3
1	A	261	VAL	2.2
5	J	207	ARG	2.2
1	F	213	ILE	2.2
4	I	151	SER	2.2
1	F	267	PRO	2.2
4	D	162	ASP	2.2
4	I	190	ASN	2.1
4	D	178	ASN	2.1
4	I	123	LEU	2.1
5	J	133	SER	2.1
5	J	206	PRO	2.1
4	I	176	TRP	2.1
5	J	203	TRP	2.1
4	I	119	ALA	2.1
4	D	136	PHE	2.1
4	I	127	LYS	2.1
1	F	222	GLU	2.1
1	A	214	THR	2.0
5	J	184	ALA	2.0
4	D	127	LYS	2.0
1	A	225	THR	2.0
4	D	130	ASP	2.0
4	I	120	VAL	2.0
4	D	184	CYS	2.0
1	A	213	ILE	2.0
4	I	124	ARG	2.0
5	J	2	ALA	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
8	SO4	J	305	5/5	0.66	0.41	75,79,97,97	0
6	EDO	F	304	4/4	0.67	0.26	62,63,72,75	0
6	EDO	I	203	4/4	0.77	0.16	39,48,50,51	0
6	EDO	F	301	4/4	0.77	0.21	55,56,57,60	0
6	EDO	J	301	4/4	0.79	0.21	65,76,76,79	0
7	GOL	D	202	6/6	0.81	0.18	49,68,70,73	0
6	EDO	G	101	4/4	0.81	0.17	52,52,54,57	0
6	EDO	E	305	4/4	0.82	0.21	48,55,56,62	0
8	SO4	F	305	5/5	0.82	0.25	96,97,104,113	0
6	EDO	E	301	4/4	0.82	0.25	59,67,69,71	0
7	GOL	A	303	6/6	0.83	0.31	38,55,56,65	0
6	EDO	F	303	4/4	0.84	0.26	43,48,51,55	0
6	EDO	I	202	4/4	0.85	0.21	53,54,60,61	0
6	EDO	E	302	4/4	0.86	0.22	50,54,55,65	0
6	EDO	E	303	4/4	0.87	0.19	61,61,64,67	0
8	SO4	E	307	5/5	0.87	0.23	62,70,80,84	0
6	EDO	B	302	4/4	0.88	0.14	58,62,63,69	0
8	SO4	E	308	5/5	0.88	0.24	74,83,92,94	0
6	EDO	I	205	4/4	0.90	0.20	34,36,39,64	0
8	SO4	J	304	5/5	0.90	0.24	77,80,82,87	0
6	EDO	I	204	4/4	0.90	0.13	43,44,45,48	0
6	EDO	A	301	4/4	0.91	0.15	49,53,65,65	0
6	EDO	A	302	4/4	0.91	0.26	46,58,64,68	0
6	EDO	F	302	4/4	0.91	0.22	39,45,45,51	0
6	EDO	C	101	4/4	0.92	0.17	37,40,42,45	0
8	SO4	D	203	5/5	0.92	0.16	84,85,91,92	0
8	SO4	D	204	5/5	0.92	0.25	72,73,82,88	0
6	EDO	B	301	4/4	0.92	0.19	43,48,51,55	0
6	EDO	B	303	4/4	0.93	0.17	48,49,53,58	0
6	EDO	E	304	4/4	0.93	0.16	35,41,44,45	0
6	EDO	J	303	4/4	0.94	0.14	35,40,41,46	0
6	EDO	I	201	4/4	0.95	0.13	40,46,47,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	D	201	4/4	0.96	0.14	41,43,47,48	0
6	EDO	J	302	4/4	0.96	0.16	34,39,45,49	0
7	GOL	E	306	6/6	0.97	0.14	39,42,43,52	0

6.5 Other polymers (i)

There are no such residues in this entry.