



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:21 PM UTC

PDB ID : 3UTS / pdb\_00003uts  
Title : 1E6-A\*0201-ALWGPDPA AAA Complex, Monoclinic  
Authors : Rizkallah, P.J.; Cole, D.K.; Sewell, A.K.; Bulek, A.M.  
Deposited on : 2011-11-26  
Resolution : 2.71 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](mailto: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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

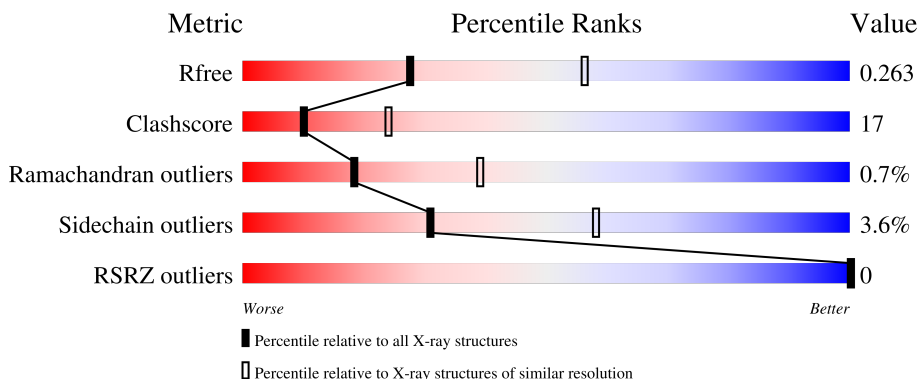
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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))
$R_{free}$	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	71% (green), 27% (yellow), 2% (red), 0% (orange), 0% (grey)
1	F	276	75% (green), 23% (yellow), 2% (red), 0% (orange), 0% (grey)
2	B	100	85% (green), 14% (yellow), 1% (red), 0% (orange), 0% (grey)
2	G	100	77% (green), 23% (yellow), 0% (red), 0% (orange), 0% (grey)
3	C	10	60% (green), 40% (yellow), 0% (red), 0% (orange), 0% (grey)

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	H	10	 90% 10%
4	D	201	 68% 26% 5%
4	I	201	 66% 27% 7%
5	E	246	 69% 29% .
5	J	246	 75% 21% .

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 13552 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
			Total	C	N	O	S			
1	A	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			
1	F	276	Total	C	N	O	S	0	1	0
			2264	1414	414	427	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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 Insulin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	10	Total	C	N	O	0	0	0
			69	45	11	13			
3	H	10	Total	C	N	O	0	0	0
			69	45	11	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	200	Total	C	N	O	S	0	0	0
			1579	989	260	320	10			

*Continued on next page...*

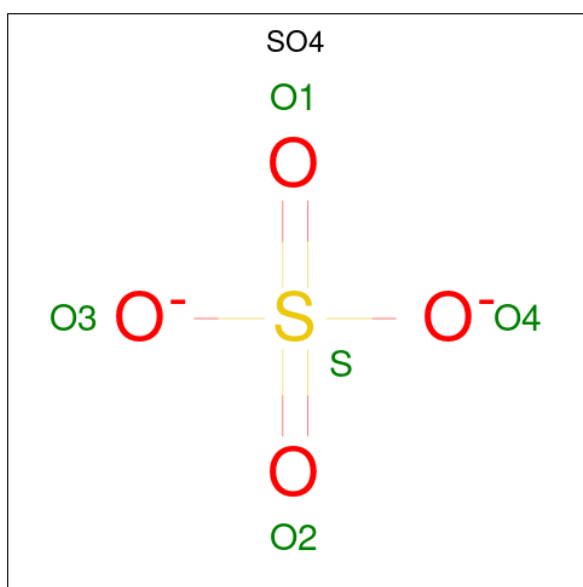
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	I	201	1586	994	261	321	10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	246	1974	1249	341	374	10	0	0	0
5	J	246	1973	1249	341	373	10	0	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0
6	D	1	5	4	1	0	0
6	F	1	5	4	1	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	C O	0	0
			6	3 3		

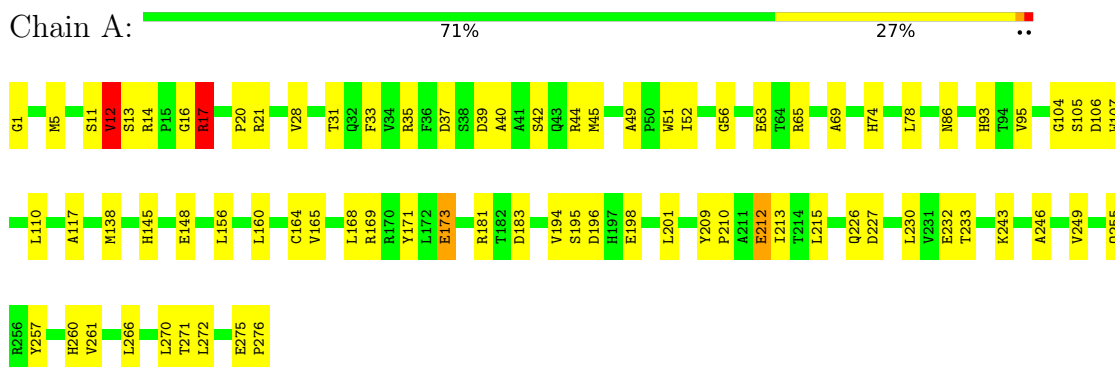
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	18	Total	O	0	0
			18	18		
8	B	10	Total	O	0	0
			10	10		
8	D	7	Total	O	0	0
			7	7		
8	E	14	Total	O	0	0
			14	14		
8	F	15	Total	O	0	0
			15	15		
8	G	5	Total	O	0	0
			5	5		
8	H	3	Total	O	0	0
			3	3		
8	I	4	Total	O	0	0
			4	4		
8	J	14	Total	O	0	0
			14	14		

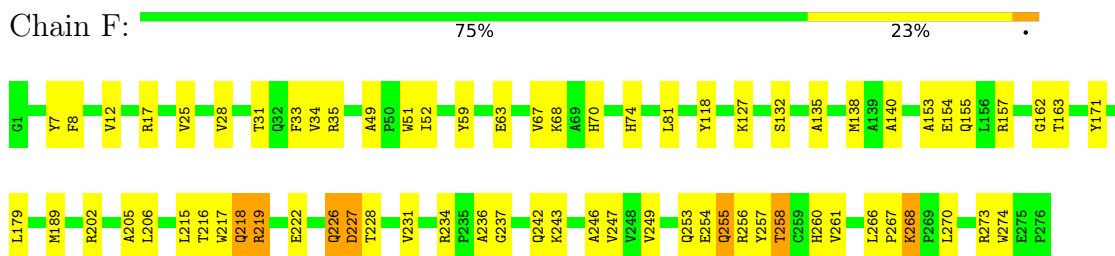
### 3 Residue-property plots

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.

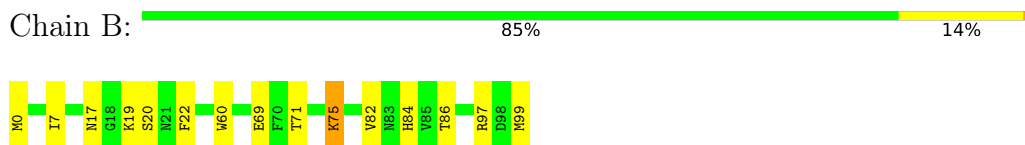
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



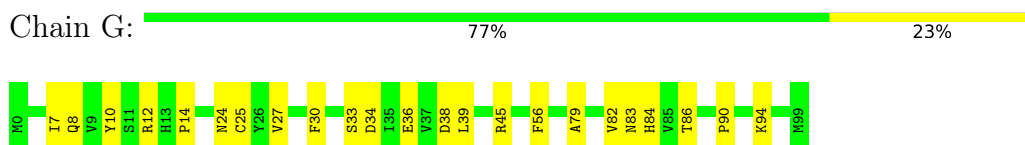
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin

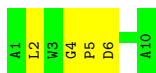


- Molecule 2: Beta-2-microglobulin




- Molecule 3: Insulin

Chain C:  60% 40%



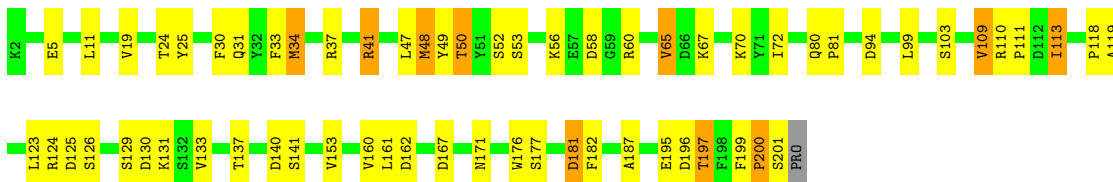
- Molecule 3: Insulin

Chain H:  90% 10%



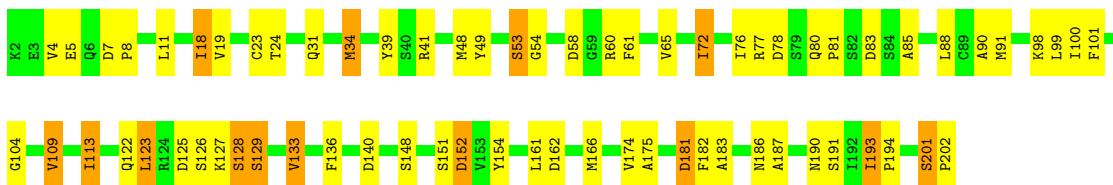
- Molecule 4: 1E6 TCR Alpha Chain

Chain D:  68% 26% 5%



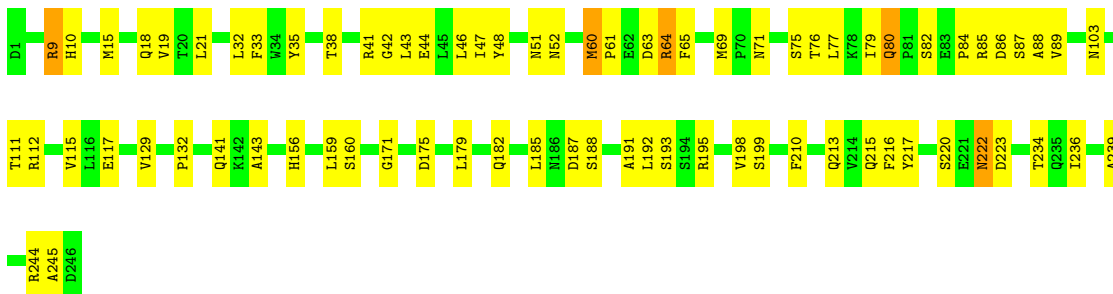
- Molecule 4: 1E6 TCR Alpha Chain

Chain I:  66% 27% 7%



- Molecule 5: 1E6 TCR Beta Chain

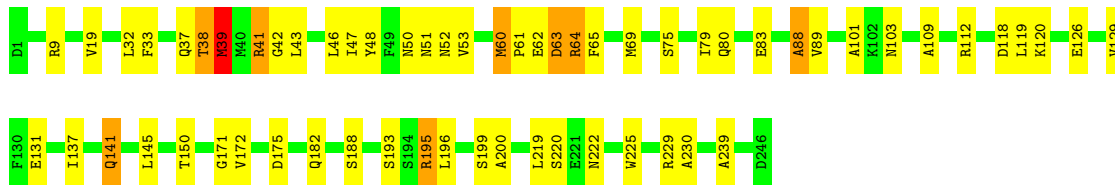
Chain E:  69% 29%



- Molecule 5: 1E6 TCR Beta Chain

Chain J:  75% 21%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.68Å 84.59Å 126.28Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	63.14 – 2.71 63.14 – 2.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (63.14-2.71) 99.2 (63.14-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.73Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.201 , 0.269 0.201 , 0.263	Depositor DCC
$R_{free}$ test set	2715 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.5	Xtrriage
Anisotropy	0.549	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 24.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.165 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: GOL, SO4

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	0.84	1/2319 (0.0%)	0.83	6/3149 (0.2%)
1	F	0.76	0/2330	0.80	1/3163 (0.0%)
2	B	0.89	0/860	0.79	0/1162
2	G	0.78	0/860	0.75	1/1162 (0.1%)
3	C	1.06	0/72	0.77	0/99
3	H	0.86	0/72	0.75	0/99
4	D	0.89	0/1615	0.86	2/2185 (0.1%)
4	I	0.93	0/1623	0.90	5/2197 (0.2%)
5	E	0.83	0/2029	0.83	1/2759 (0.0%)
5	J	0.92	0/2028	0.94	7/2759 (0.3%)
All	All	0.85	1/13808 (0.0%)	0.85	23/18734 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	VAL	CA-CB	5.84	1.61	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	63	ASP	N-CA-C	-11.20	93.78	110.24
4	I	129	SER	N-CA-C	-7.97	97.75	109.63
4	D	197	THR	N-CA-C	7.71	122.26	109.46
5	J	39	MET	N-CA-C	7.39	119.85	110.24
1	F	255	GLN	N-CA-C	-6.77	105.01	113.20
4	I	128	SER	N-CA-C	6.75	116.96	108.45
1	A	14	ARG	CA-C-N	6.63	128.13	119.84
1	A	14	ARG	C-N-CA	6.63	128.13	119.84
5	J	38	THR	N-CA-C	-6.55	98.06	108.73
5	E	245	ALA	N-CA-C	-6.27	104.50	111.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	18	ILE	CB-CA-C	-5.94	103.43	111.63
5	J	126	GLU	N-CA-C	-5.71	100.40	109.76
4	I	53	SER	N-CA-C	5.62	115.54	108.45
4	D	137	THR	N-CA-C	5.46	117.14	108.79
5	J	150	THR	N-CA-C	5.37	117.34	109.24
4	I	72	ILE	CB-CA-C	-5.33	103.26	111.31
2	G	56	PHE	N-CA-C	5.25	117.06	109.07
1	A	45	MET	N-CA-C	-5.25	102.09	109.96
1	A	17	ARG	N-CA-C	5.06	116.14	107.28
1	A	56	GLY	CA-C-N	5.05	124.83	119.28
1	A	56	GLY	C-N-CA	5.05	124.83	119.28
5	J	83	GLU	CA-C-N	5.01	124.45	119.24
5	J	83	GLU	C-N-CA	5.01	124.45	119.24

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	2253	0	2103	70	0
1	F	2264	0	2115	83	0
2	B	837	0	803	14	0
2	G	837	0	803	17	0
3	C	69	0	64	3	0
3	H	69	0	64	3	0
4	D	1579	0	1494	71	0
4	I	1586	0	1501	82	0
5	E	1974	0	1887	74	0
5	J	1973	0	1887	70	0
6	A	5	0	0	1	0
6	D	5	0	0	0	0
6	F	5	0	0	1	0
7	J	6	0	8	0	0
8	A	18	0	0	3	0
8	B	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	D	7	0	0	2	0
8	E	14	0	0	2	0
8	F	15	0	0	0	0
8	G	5	0	0	0	0
8	H	3	0	0	0	0
8	I	4	0	0	0	0
8	J	14	0	0	0	0
All	All	13552	0	12729	453	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 17.

All (453) 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:F:266:LEU:HD22	1:F:270:LEU:CD1	1.62	1.28
1:F:266:LEU:CD2	1:F:270:LEU:HD12	1.66	1.24
1:F:266:LEU:HD23	1:F:270:LEU:HD12	1.31	1.11
4:D:33:PHE:CD1	4:D:72:ILE:HD11	1.90	1.06
1:F:266:LEU:CD2	1:F:270:LEU:CD1	2.27	1.05
1:F:266:LEU:HD22	1:F:270:LEU:HD11	1.36	1.04
4:D:113:ILE:HD13	4:D:113:ILE:H	1.24	1.01
4:I:113:ILE:HD13	4:I:113:ILE:H	1.21	1.01
5:E:46:LEU:HB3	5:E:60:MET:HE3	1.46	0.96
4:I:19:VAL:CG1	4:I:76:ILE:HB	1.96	0.96
1:F:226:GLN:HE21	1:F:226:GLN:HA	1.32	0.95
5:E:129:VAL:HG23	5:E:239:ALA:CB	1.97	0.94
1:F:189:MET:SD	1:F:274:TRP:HB2	2.08	0.93
1:F:218:GLN:HB2	1:F:258:THR:HG23	1.50	0.92
5:E:15:MET:HE3	5:E:117:GLU:HA	1.51	0.92
4:I:34:MET:HE2	5:J:103:ASN:HB2	1.51	0.90
4:I:136:PHE:CZ	4:I:193:ILE:CG2	2.56	0.89
4:I:136:PHE:CZ	4:I:193:ILE:HG23	2.08	0.88
5:J:38:THR:O	5:J:41:ARG:HB3	1.73	0.87
5:J:41:ARG:HG2	5:J:41:ARG:HH11	1.39	0.87
4:I:161:LEU:HD21	5:J:171:GLY:O	1.75	0.86
4:I:193:ILE:HG22	4:I:194:PRO:HD2	1.58	0.86
5:J:60:MET:HE2	5:J:61:PRO:HD2	1.56	0.85
1:F:138:MET:HE2	1:F:138:MET:HA	1.58	0.84
5:E:129:VAL:HG23	5:E:239:ALA:HB3	1.59	0.83
5:E:64:ARG:NH2	5:E:86:ASP:OD1	2.11	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:197:THR:OG1	4:D:199:PHE:CZ	2.33	0.81
4:I:34:MET:HE3	4:I:49:TYR:HB2	1.62	0.81
1:F:243:LYS:NZ	6:F:277:SO4:O4	2.11	0.81
5:J:41:ARG:HG3	5:J:42:GLY:O	1.81	0.80
2:B:20:SER:HA	2:B:71:THR:HG22	1.63	0.80
4:I:48:MET:HE2	4:I:61:PHE:HB2	1.65	0.79
1:A:17:ARG:HG3	1:A:17:ARG:HH11	1.47	0.79
5:J:64:ARG:HB2	5:J:80:GLN:O	1.82	0.79
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.64	0.78
4:I:80:GLN:O	4:I:109:VAL:HG11	1.84	0.78
1:F:273:ARG:HH11	1:F:273:ARG:HG2	1.48	0.78
5:E:179:LEU:HD23	5:E:191:ALA:O	1.85	0.77
1:F:218:GLN:CB	1:F:258:THR:HG23	2.13	0.77
1:F:33:PHE:CD2	1:F:34:VAL:HG13	2.20	0.77
4:D:41:ARG:HH11	4:D:41:ARG:CG	1.98	0.77
5:E:129:VAL:HG23	5:E:239:ALA:HB1	1.65	0.76
4:I:5:GLU:HB3	4:I:24:THR:CG2	2.16	0.76
1:F:218:GLN:HG3	1:F:260:HIS:NE2	1.99	0.76
1:F:226:GLN:HE21	1:F:226:GLN:CA	1.99	0.76
4:I:60:ARG:NH2	4:I:83:ASP:OD2	2.18	0.76
5:J:9:ARG:NH1	5:J:109:ALA:HB3	2.01	0.76
5:J:32:LEU:HD23	5:J:32:LEU:C	2.11	0.76
1:A:266:LEU:HD12	1:A:266:LEU:O	1.86	0.75
5:E:42:GLY:HA2	8:E:255:HOH:O	1.86	0.75
1:A:249:VAL:HG12	1:A:257:TYR:CZ	2.20	0.75
5:J:32:LEU:HD23	5:J:33:PHE:N	2.01	0.75
5:J:62:GLU:OE2	5:J:62:GLU:N	2.20	0.75
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.17	0.75
1:A:63:GLU:OE1	3:C:2:LEU:HB2	1.87	0.74
5:E:21:LEU:HD22	5:E:111:THR:HG21	1.68	0.74
5:E:175:ASP:OD2	5:E:193:SER:HB3	1.87	0.74
4:I:72:ILE:HD11	4:I:91:MET:CE	2.17	0.74
4:D:34:MET:HE2	5:E:103:ASN:HB2	1.70	0.73
4:I:34:MET:HE1	5:J:103:ASN:ND2	2.04	0.73
4:D:160:VAL:HG22	4:D:171:ASN:ND2	2.03	0.72
4:I:34:MET:HE2	5:J:103:ASN:CB	2.19	0.72
1:A:266:LEU:HD22	1:A:270:LEU:HD13	1.72	0.72
5:J:141:GLN:HE21	5:J:141:GLN:HA	1.55	0.72
4:I:161:LEU:HD21	5:J:171:GLY:C	2.15	0.71
5:E:159:LEU:HD23	5:E:160:SER:N	2.05	0.71
5:J:141:GLN:HE21	5:J:141:GLN:CA	2.01	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:113:ILE:HG13	4:D:140:ASP:HA	1.71	0.71
5:J:46:LEU:HB3	5:J:60:MET:HE3	1.73	0.71
4:D:48:MET:HA	4:D:48:MET:HE2	1.73	0.71
4:D:81:PRO:HA	4:D:109:VAL:HG13	1.71	0.71
4:I:193:ILE:CG2	4:I:194:PRO:HD2	2.21	0.70
4:D:113:ILE:H	4:D:113:ILE:CD1	2.01	0.70
4:I:72:ILE:HD11	4:I:91:MET:HE1	1.74	0.70
4:I:5:GLU:HB3	4:I:24:THR:HG23	1.74	0.69
1:A:17:ARG:HH11	1:A:17:ARG:CG	2.05	0.69
4:I:34:MET:HE3	4:I:49:TYR:CB	2.24	0.68
4:I:113:ILE:H	4:I:113:ILE:CD1	2.02	0.68
1:F:138:MET:HE2	1:F:138:MET:CA	2.23	0.68
4:I:81:PRO:HA	4:I:109:VAL:HG13	1.74	0.68
4:I:113:ILE:HD13	4:I:113:ILE:N	2.03	0.68
4:I:148:SER:HA	4:I:190:ASN:HD22	1.58	0.68
1:F:217:TRP:CD1	1:F:247:VAL:HG13	2.29	0.67
5:J:172:VAL:HG22	5:J:196:LEU:HD13	1.76	0.67
4:D:133:VAL:HG23	4:D:176:TRP:HB3	1.77	0.67
1:F:256:ARG:HD2	1:F:256:ARG:O	1.95	0.67
4:D:33:PHE:CD1	4:D:72:ILE:CD1	2.76	0.67
5:E:19:VAL:HG22	5:E:79:ILE:HB	1.77	0.67
5:E:63:ASP:O	5:E:64:ARG:HG3	1.95	0.67
4:I:48:MET:CE	4:I:58:ASP:HB3	2.25	0.66
4:D:41:ARG:HH11	4:D:41:ARG:HG2	1.61	0.66
4:I:182:PHE:CZ	4:I:187:ALA:HB2	2.31	0.66
5:J:129:VAL:HG23	5:J:239:ALA:HB3	1.78	0.66
5:E:195:ARG:HD2	5:E:195:ARG:N	2.11	0.66
1:F:266:LEU:HD12	1:F:267:PRO:HD2	1.76	0.66
4:D:80:GLN:O	4:D:109:VAL:HG11	1.95	0.65
5:J:60:MET:HE2	5:J:60:MET:HA	1.77	0.65
4:D:110:ARG:HB3	4:D:141:SER:HB3	1.79	0.65
1:A:271:THR:C	1:A:272:LEU:HD12	2.22	0.64
4:D:161:LEU:HD21	5:E:171:GLY:C	2.22	0.64
1:F:218:GLN:HG3	1:F:260:HIS:CD2	2.33	0.64
4:I:133:VAL:HG13	4:I:174:VAL:HG13	1.80	0.64
5:J:63:ASP:O	5:J:65:PHE:N	2.31	0.64
5:E:179:LEU:HD23	5:E:179:LEU:H	1.63	0.64
1:F:216:THR:OG1	1:F:260:HIS:HB2	1.98	0.64
4:D:118:PRO:O	4:D:196:ASP:HB2	1.98	0.64
4:D:113:ILE:HD13	4:D:113:ILE:N	2.06	0.63
4:D:123:LEU:HD22	5:E:132:PRO:HA	1.80	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:62:GLU:O	5:J:63:ASP:C	2.41	0.63
1:F:266:LEU:CD2	1:F:268:LYS:O	2.46	0.63
1:A:260:HIS:CD2	1:A:271:THR:HG22	2.33	0.63
5:J:19:VAL:HG22	5:J:79:ILE:HB	1.79	0.63
5:J:172:VAL:CG2	5:J:196:LEU:HD13	2.28	0.63
5:J:175:ASP:OD2	5:J:193:SER:HB3	1.98	0.63
5:E:60:MET:HE2	5:E:60:MET:HA	1.82	0.62
4:I:113:ILE:HG13	4:I:140:ASP:HA	1.81	0.62
1:F:228:THR:CG2	1:F:247:VAL:HG12	2.30	0.61
5:E:182:GLN:NE2	5:E:185:LEU:HD22	2.15	0.61
4:D:34:MET:HE2	5:E:103:ASN:CB	2.31	0.61
4:D:161:LEU:HD13	4:D:162:ASP:N	2.15	0.61
5:E:32:LEU:HD13	5:E:75:SER:HB2	1.82	0.61
4:D:119:ALA:HB2	4:D:197:THR:CG2	2.31	0.61
4:I:136:PHE:HZ	4:I:193:ILE:HG23	1.64	0.60
1:A:16:GLY:C	1:A:17:ARG:HD3	2.26	0.60
4:D:197:THR:OG1	4:D:199:PHE:CE2	2.55	0.60
1:A:181:ARG:NH1	1:A:183:ASP:OD2	2.34	0.60
5:J:137:ILE:O	5:J:141:GLN:NE2	2.35	0.60
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.37	0.60
4:D:119:ALA:CB	4:D:197:THR:CG2	2.80	0.60
2:B:20:SER:CA	2:B:71:THR:HG22	2.33	0.59
1:A:49:ALA:O	1:A:52:ILE:HG22	2.03	0.59
1:A:212:GLU:C	1:A:212:GLU:OE1	2.46	0.59
4:I:11:LEU:HD12	4:I:11:LEU:O	2.03	0.59
5:J:38:THR:HG22	5:J:88:ALA:HB2	1.85	0.59
4:D:103:SER:HB2	8:D:206:HOH:O	2.03	0.59
5:E:61:PRO:HG2	5:E:65:PHE:CD1	2.37	0.59
5:E:60:MET:HE2	5:E:61:PRO:HD2	1.84	0.59
1:F:218:GLN:O	1:F:258:THR:N	2.36	0.59
1:F:266:LEU:HD22	1:F:270:LEU:CG	2.32	0.58
1:F:70:HIS:O	1:F:74:HIS:HD2	1.85	0.58
4:I:72:ILE:CD1	4:I:91:MET:HE1	2.33	0.58
4:I:166:MET:HE1	5:J:199:SER:HB3	1.85	0.58
4:D:37:ARG:HB2	4:D:47:LEU:HD11	1.86	0.58
5:E:129:VAL:CG2	5:E:239:ALA:HB3	2.31	0.58
4:I:152:ASP:N	4:I:152:ASP:OD1	2.35	0.58
4:I:19:VAL:HG12	4:I:76:ILE:HB	1.82	0.58
5:J:229:ARG:O	5:J:230:ALA:C	2.45	0.58
5:E:179:LEU:HD21	5:E:191:ALA:HB3	1.85	0.57
1:F:266:LEU:HD21	1:F:268:LYS:O	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:34:MET:CE	4:I:49:TYR:HB2	2.34	0.57
4:D:160:VAL:HG22	4:D:171:ASN:HD21	1.68	0.57
1:F:7:TYR:CE2	3:H:2:LEU:CD1	2.88	0.57
4:I:19:VAL:HG11	4:I:76:ILE:HB	1.85	0.57
4:I:193:ILE:HG22	4:I:194:PRO:CD	2.33	0.57
5:J:137:ILE:HG23	5:J:200:ALA:HB1	1.87	0.57
4:D:125:ASP:OD1	4:D:126:SER:N	2.37	0.57
4:D:161:LEU:HD21	5:E:171:GLY:O	2.05	0.57
4:I:72:ILE:CD1	4:I:91:MET:CE	2.83	0.57
1:F:218:GLN:CG	1:F:260:HIS:CD2	2.87	0.57
5:E:38:THR:HG22	5:E:88:ALA:HB2	1.87	0.56
5:J:119:LEU:HD22	5:J:219:LEU:HD21	1.87	0.56
4:D:125:ASP:CB	4:D:131:LYS:HB2	2.35	0.56
5:J:41:ARG:HH11	5:J:41:ARG:CG	2.15	0.56
4:D:33:PHE:HB3	4:D:72:ILE:HD13	1.86	0.56
5:E:41:ARG:HD3	5:E:44:GLU:OE2	2.05	0.56
1:F:234:ARG:HD2	2:G:10:TYR:CE1	2.40	0.56
1:F:236:ALA:HB2	1:F:242:GLN:HG3	1.86	0.56
4:D:52:SER:HA	4:D:67:LYS:HE2	1.87	0.56
4:I:88:LEU:HD23	4:I:104:GLY:HA3	1.86	0.56
4:I:161:LEU:CD2	5:J:171:GLY:C	2.78	0.56
4:I:88:LEU:HD23	4:I:104:GLY:CA	2.36	0.56
4:I:136:PHE:HZ	4:I:193:ILE:CG2	2.17	0.56
5:J:32:LEU:C	5:J:32:LEU:CD2	2.79	0.56
4:I:48:MET:HE1	4:I:58:ASP:HB3	1.88	0.56
1:F:226:GLN:HA	1:F:226:GLN:NE2	2.12	0.56
5:E:132:PRO:HG2	5:E:143:ALA:HB1	1.87	0.55
1:A:1:GLY:O	1:A:105:SER:HA	2.05	0.55
1:A:12:VAL:HG13	1:A:21:ARG:HB3	1.88	0.55
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.42	0.55
5:E:9:ARG:HD3	5:E:10:HIS:CD2	2.42	0.55
4:D:34:MET:HE3	4:D:49:TYR:HB2	1.87	0.55
1:F:219:ARG:C	1:F:219:ARG:HD2	2.32	0.55
1:A:11:SER:HB3	1:A:95:VAL:HG22	1.89	0.55
4:I:136:PHE:CZ	4:I:193:ILE:HG21	2.41	0.55
1:A:160:LEU:HA	1:A:164:CYS:SG	2.48	0.54
1:F:236:ALA:HB2	1:F:242:GLN:CG	2.37	0.54
4:I:90:ALA:HB2	4:I:101:PHE:CD1	2.42	0.54
4:D:119:ALA:CB	4:D:197:THR:HG23	2.38	0.54
1:F:28:VAL:HG23	1:F:33:PHE:CD1	2.42	0.54
1:F:226:GLN:O	1:F:227:ASP:CB	2.55	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:GLY:H	2:G:24:ASN:HD21	1.56	0.54
1:A:17:ARG:HD3	1:A:17:ARG:N	2.23	0.54
1:A:104:GLY:HA2	1:A:110:LEU:HD11	1.88	0.54
5:J:60:MET:HA	5:J:60:MET:CE	2.38	0.54
2:G:79:ALA:HB2	2:G:94:LYS:HA	1.90	0.53
4:I:126:SER:O	4:I:127:LYS:C	2.48	0.53
2:G:38:ASP:OD1	2:G:45:ARG:NE	2.39	0.53
5:E:87:SER:HB3	5:E:115:VAL:H	1.73	0.53
4:I:98:LYS:HE2	4:I:100:ILE:HD11	1.90	0.53
5:E:175:ASP:HB2	5:E:192:LEU:HD12	1.89	0.53
5:J:32:LEU:HD13	5:J:75:SER:HB2	1.90	0.53
4:I:48:MET:HE1	4:I:58:ASP:CB	2.38	0.53
1:F:127:LYS:HD3	1:F:132:SER:OG	2.08	0.53
1:F:51:TRP:CZ2	1:F:179:LEU:HD11	2.44	0.53
4:I:182:PHE:CE1	4:I:187:ALA:HB2	2.43	0.53
5:J:89:VAL:HG22	5:J:112:ARG:HG2	1.91	0.53
2:B:75:LYS:CG	2:B:75:LYS:O	2.56	0.53
5:E:15:MET:CE	5:E:117:GLU:HG2	2.38	0.53
5:E:159:LEU:HD23	5:E:159:LEU:C	2.34	0.53
4:I:11:LEU:HD12	4:I:11:LEU:C	2.33	0.53
4:D:113:ILE:O	4:D:113:ILE:HG12	2.09	0.52
1:F:7:TYR:CZ	3:H:2:LEU:HD12	2.44	0.52
4:D:119:ALA:HB1	4:D:197:THR:HG23	1.92	0.52
4:I:201:SER:O	4:I:202:PRO:C	2.53	0.52
1:A:65:ARG:HD3	8:A:281:HOH:O	2.10	0.52
1:F:135:ALA:HB1	1:F:140:ALA:HB3	1.92	0.52
4:I:41:ARG:HH12	5:J:112:ARG:NH1	2.07	0.52
4:I:154:TYR:O	4:I:175:ALA:HA	2.10	0.52
1:A:212:GLU:OE1	1:A:213:ILE:N	2.43	0.52
4:D:41:ARG:CG	4:D:41:ARG:NH1	2.67	0.52
5:E:21:LEU:HD12	5:E:77:LEU:HD23	1.91	0.52
1:F:231:VAL:HB	2:G:8:GLN:HE22	1.74	0.52
4:I:122:GLN:C	4:I:123:LEU:HD12	2.34	0.52
1:A:138:MET:HE2	1:A:138:MET:HA	1.92	0.52
4:D:153:VAL:HA	4:D:177:SER:OG	2.11	0.51
5:E:182:GLN:HE21	5:E:185:LEU:HD22	1.75	0.51
1:F:67:VAL:HG13	1:F:68:LYS:N	2.25	0.51
5:J:141:GLN:HE21	5:J:141:GLN:N	2.07	0.51
1:F:228:THR:HG21	1:F:247:VAL:HG12	1.91	0.51
2:B:99:MET:HG3	2:B:99:MET:O	2.11	0.51
5:E:63:ASP:C	5:E:64:ARG:CG	2.84	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:GLU:OE1	1:F:154:GLU:HA	2.10	0.51
1:F:249:VAL:HG12	1:F:257:TYR:CZ	2.46	0.51
5:J:37:GLN:HB2	5:J:43:LEU:CD2	2.41	0.51
4:D:181:ASP:N	4:D:181:ASP:OD1	2.42	0.51
5:E:19:VAL:CG2	5:E:79:ILE:HB	2.41	0.50
2:G:79:ALA:CB	2:G:94:LYS:HA	2.42	0.50
4:I:34:MET:CE	5:J:103:ASN:ND2	2.73	0.50
2:B:7:ILE:HD11	2:B:82:VAL:HB	1.93	0.50
1:F:67:VAL:CG1	1:F:68:LYS:N	2.73	0.50
1:A:65:ARG:NH1	8:A:281:HOH:O	2.42	0.50
2:B:17:ASN:OD1	2:B:97:ARG:NH2	2.45	0.50
1:F:138:MET:HA	1:F:138:MET:CE	2.38	0.50
1:F:205:ALA:C	1:F:206:LEU:HD12	2.37	0.50
1:F:237:GLY:HA3	2:G:12:ARG:NE	2.27	0.50
1:A:74:HIS:HD1	1:A:95:VAL:HG23	1.77	0.50
4:D:53:SER:HA	4:D:65:VAL:HG13	1.92	0.50
2:G:7:ILE:HD13	2:G:82:VAL:CG2	2.41	0.50
1:A:93:HIS:CD2	2:B:0:MET:HE1	2.47	0.50
4:D:41:ARG:HH11	4:D:41:ARG:HG3	1.75	0.50
4:D:5:GLU:HB3	4:D:24:THR:CG2	2.41	0.49
5:J:141:GLN:CA	5:J:141:GLN:NE2	2.71	0.49
5:J:225:TRP:NE1	5:J:229:ARG:O	2.45	0.49
4:D:34:MET:HE1	5:E:103:ASN:ND2	2.27	0.49
4:D:52:SER:HA	4:D:67:LYS:CE	2.42	0.49
5:J:46:LEU:HD22	5:J:60:MET:CE	2.42	0.49
1:A:169:ARG:NH2	6:A:277:SO4:O4	2.45	0.49
1:F:217:TRP:CD1	1:F:247:VAL:CG1	2.95	0.49
5:E:222:ASN:HD22	5:E:223:ASP:N	2.10	0.49
1:F:7:TYR:CE2	3:H:2:LEU:HD12	2.47	0.49
5:J:50:ASN:O	5:J:53:VAL:HG22	2.13	0.49
4:D:11:LEU:HD11	4:D:19:VAL:HG21	1.94	0.48
5:E:15:MET:HE2	5:E:84:PRO:HD3	1.94	0.48
5:E:69:MET:HE2	5:E:71:ASN:O	2.13	0.48
5:J:46:LEU:HD22	5:J:60:MET:HE3	1.94	0.48
4:D:41:ARG:HG2	4:D:41:ARG:NH1	2.27	0.48
1:F:8:PHE:HB2	1:F:25:VAL:HG22	1.94	0.48
1:F:135:ALA:HB1	1:F:140:ALA:CB	2.43	0.48
4:I:123:LEU:HD12	4:I:123:LEU:N	2.28	0.48
4:D:52:SER:O	4:D:65:VAL:HG11	2.13	0.48
4:I:53:SER:OG	4:I:54:GLY:N	2.45	0.48
1:A:249:VAL:CG1	1:A:257:TYR:CZ	2.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:193:ILE:HD12	4:I:193:ILE:H	1.78	0.48
1:A:37:ASP:OD1	1:A:39:ASP:N	2.44	0.48
1:A:196:ASP:OD1	1:A:196:ASP:O	2.32	0.48
1:A:117:ALA:HB2	2:B:60:TRP:CZ2	2.49	0.48
1:A:37:ASP:OD1	1:A:37:ASP:C	2.57	0.48
1:A:160:LEU:O	1:A:165:VAL:HG23	2.13	0.48
2:B:99:MET:O	2:B:99:MET:CG	2.62	0.48
5:E:213:GLN:HG3	5:E:236:ILE:CG2	2.44	0.48
1:F:138:MET:HE2	1:F:138:MET:N	2.28	0.48
1:F:217:TRP:NE1	1:F:247:VAL:HG13	2.28	0.48
4:I:113:ILE:HD11	4:I:140:ASP:HB2	1.95	0.48
1:F:31:THR:HG21	1:F:179:LEU:CD2	2.44	0.48
4:I:19:VAL:HG12	4:I:76:ILE:O	2.14	0.48
4:I:23:CYS:HB2	4:I:72:ILE:HD12	1.96	0.48
2:B:84:HIS:CE1	2:B:86:THR:HG23	2.49	0.47
1:F:219:ARG:O	1:F:222:GLU:HB2	2.13	0.47
1:A:104:GLY:CA	1:A:110:LEU:HD11	2.44	0.47
2:B:75:LYS:O	2:B:75:LYS:HG2	2.12	0.47
4:D:34:MET:CE	4:D:49:TYR:HB2	2.43	0.47
4:D:125:ASP:HB2	4:D:131:LYS:HB2	1.96	0.47
5:E:32:LEU:HD23	5:E:32:LEU:C	2.39	0.47
4:I:136:PHE:CE1	4:I:193:ILE:HG21	2.50	0.47
1:A:249:VAL:HG12	1:A:257:TYR:CE1	2.50	0.47
1:A:74:HIS:HD1	1:A:95:VAL:CG2	2.27	0.47
1:A:215:LEU:HD21	1:A:261:VAL:HG22	1.93	0.47
1:A:266:LEU:CD2	1:A:270:LEU:HD13	2.44	0.47
4:D:5:GLU:HB3	4:D:24:THR:HG23	1.97	0.47
4:D:11:LEU:O	4:D:11:LEU:HD12	2.15	0.47
5:E:15:MET:HE1	5:E:117:GLU:HG2	1.95	0.47
5:E:132:PRO:CG	5:E:143:ALA:HB1	2.44	0.47
5:E:213:GLN:HG3	5:E:236:ILE:HG23	1.97	0.47
1:F:218:GLN:N	1:F:258:THR:O	2.43	0.47
1:F:237:GLY:H	2:G:24:ASN:ND2	2.12	0.47
4:I:7:ASP:OD1	4:I:8:PRO:HD2	2.15	0.47
5:J:129:VAL:HG23	5:J:239:ALA:CB	2.41	0.47
5:J:182:GLN:O	5:J:188:SER:HB2	2.15	0.47
1:A:106:ASP:O	1:A:107:TRP:HB2	2.16	0.46
5:E:89:VAL:HG22	5:E:112:ARG:HG2	1.97	0.46
1:F:49:ALA:O	1:F:52:ILE:HG22	2.14	0.46
1:A:40:ALA:HB3	8:A:283:HOH:O	2.16	0.46
1:A:230:LEU:HD11	1:A:243:LYS:HE3	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:PRO:HG3	4:D:160:VAL:HG21	1.96	0.46
4:I:48:MET:HE1	4:I:58:ASP:N	2.30	0.46
1:F:253:GLN:N	1:F:253:GLN:OE1	2.49	0.46
2:G:33:SER:O	2:G:34:ASP:C	2.58	0.46
4:D:195:GLU:OE2	4:D:195:GLU:HA	2.15	0.46
5:E:21:LEU:CD2	5:E:111:THR:HG21	2.42	0.46
4:I:128:SER:OG	4:I:129:SER:O	2.19	0.46
1:A:42:SER:O	1:A:44:ARG:HG2	2.16	0.46
1:F:273:ARG:HG2	1:F:273:ARG:NH1	2.23	0.46
4:I:48:MET:CE	4:I:61:PHE:HB2	2.41	0.46
1:F:70:HIS:O	1:F:74:HIS:CD2	2.68	0.46
2:G:25:CYS:HB2	2:G:39:LEU:HD21	1.98	0.46
1:A:201:LEU:O	1:A:246:ALA:HA	2.16	0.45
5:E:32:LEU:HD23	5:E:33:PHE:N	2.31	0.45
1:A:173:GLU:OE1	1:A:173:GLU:N	2.49	0.45
5:E:84:PRO:C	5:E:86:ASP:H	2.23	0.45
5:J:171:GLY:O	5:J:196:LEU:HD12	2.16	0.45
4:D:124:ARG:NH1	8:D:207:HOH:O	2.49	0.45
5:E:216:PHE:O	5:E:234:THR:HG23	2.16	0.45
5:J:51:ASN:O	5:J:52:ASN:HB2	2.17	0.45
4:I:181:ASP:N	4:I:181:ASP:OD1	2.50	0.45
5:E:179:LEU:CD2	5:E:191:ALA:O	2.60	0.45
4:I:126:SER:HB3	5:J:131:GLU:OE2	2.16	0.45
5:J:63:ASP:O	5:J:64:ARG:C	2.59	0.45
5:J:195:ARG:HD2	5:J:195:ARG:N	2.31	0.45
5:J:41:ARG:HG2	5:J:41:ARG:NH1	2.18	0.45
4:D:11:LEU:HD12	4:D:11:LEU:C	2.42	0.45
4:I:34:MET:CE	5:J:103:ASN:CG	2.89	0.45
4:I:183:ALA:O	4:I:186:ASN:HB3	2.17	0.45
1:A:51:TRP:CZ3	1:A:171:TYR:HB3	2.52	0.44
1:A:194:VAL:O	1:A:198:GLU:O	2.34	0.44
5:E:19:VAL:HG13	5:E:82:SER:OG	2.17	0.44
1:F:28:VAL:HG21	1:F:51:TRP:HH2	1.82	0.44
5:J:118:ASP:OD1	5:J:120:LYS:HG2	2.16	0.44
1:A:69:ALA:HB1	3:C:6:ASP:HB3	1.99	0.44
1:A:209:TYR:HA	1:A:210:PRO:C	2.43	0.44
1:F:255:GLN:C	1:F:257:TYR:H	2.24	0.44
5:J:41:ARG:CG	5:J:41:ARG:NH1	2.77	0.44
5:E:215:GLN:NE2	8:E:256:HOH:O	2.46	0.44
1:F:59:TYR:O	1:F:63:GLU:HG2	2.18	0.44
1:F:254:GLU:C	1:F:256:ARG:H	2.26	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:60:MET:HE2	5:J:61:PRO:CD	2.36	0.44
1:A:215:LEU:HD23	1:A:261:VAL:HG22	1.97	0.44
4:D:48:MET:HE1	4:D:58:ASP:HB2	2.00	0.44
4:I:5:GLU:CB	4:I:24:THR:HG23	2.45	0.44
4:I:161:LEU:HD13	4:I:162:ASP:N	2.32	0.44
5:J:141:GLN:NE2	5:J:141:GLN:N	2.66	0.44
1:A:5:MET:CE	1:A:164:CYS:HB2	2.48	0.44
1:A:13:SER:HA	1:A:20:PRO:HB3	1.99	0.44
4:D:167:ASP:OD2	4:D:167:ASP:C	2.60	0.44
1:A:93:HIS:HD2	2:B:0:MET:HE1	1.83	0.43
2:G:7:ILE:HD11	2:G:82:VAL:HB	2.00	0.43
4:D:34:MET:CE	5:E:103:ASN:CG	2.92	0.43
4:D:119:ALA:HB2	4:D:197:THR:HG22	1.98	0.43
5:E:47:ILE:HG12	5:E:48:TYR:N	2.32	0.43
5:E:187:ASP:O	5:E:188:SER:C	2.60	0.43
5:J:61:PRO:C	5:J:62:GLU:OE2	2.61	0.43
1:F:162:GLY:O	1:F:163:THR:C	2.60	0.43
5:J:37:GLN:HB2	5:J:43:LEU:HD23	2.01	0.43
1:A:255:GLN:OE1	1:A:255:GLN:N	2.51	0.43
1:F:33:PHE:CE2	1:F:34:VAL:HG13	2.54	0.43
1:F:81:LEU:HD23	1:F:118:TYR:CG	2.53	0.43
1:F:231:VAL:HB	2:G:8:GLN:NE2	2.34	0.43
2:G:36:GLU:HB3	2:G:83:ASN:HB3	2.01	0.43
1:A:156:LEU:HD23	1:A:156:LEU:HA	1.87	0.43
4:D:182:PHE:CE1	4:D:187:ALA:HB2	2.54	0.43
1:F:153:ALA:O	1:F:157:ARG:HB2	2.19	0.43
1:A:249:VAL:CG1	1:A:257:TYR:CE2	3.01	0.43
5:E:63:ASP:O	5:E:64:ARG:CG	2.65	0.43
5:E:179:LEU:H	5:E:179:LEU:CD2	2.29	0.43
5:E:51:ASN:O	5:E:52:ASN:HB2	2.19	0.43
4:I:72:ILE:CD1	4:I:91:MET:HE2	2.49	0.43
4:D:31:GLN:NE2	4:D:94:ASP:HB3	2.34	0.42
4:D:50:THR:HG23	4:D:56:LYS:HD3	2.02	0.42
4:D:195:GLU:OE2	4:D:195:GLU:CA	2.67	0.42
1:F:155:GLN:OE1	5:J:101:ALA:HB1	2.19	0.42
4:I:48:MET:HE2	4:I:58:ASP:HB3	2.00	0.42
5:E:84:PRO:O	5:E:86:ASP:N	2.53	0.42
5:E:220:SER:OG	5:E:222:ASN:ND2	2.52	0.42
1:F:215:LEU:HD22	1:F:261:VAL:HG22	2.01	0.42
5:J:220:SER:OG	5:J:222:ASN:OD1	2.30	0.42
1:A:17:ARG:CG	1:A:17:ARG:NH1	2.75	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:GLN:HA	1:F:222:GLU:O	2.19	0.42
4:D:200:PRO:O	4:D:201:SER:OG	2.35	0.42
1:F:219:ARG:O	1:F:219:ARG:CD	2.67	0.42
4:D:30:PHE:O	4:D:67:LYS:NZ	2.53	0.42
4:D:118:PRO:HB2	4:D:196:ASP:HB3	2.01	0.42
1:A:194:VAL:HG12	1:A:195:SER:OG	2.18	0.42
5:E:198:VAL:HG23	5:E:199:SER:O	2.19	0.42
5:J:63:ASP:O	5:J:65:PHE:HD1	2.03	0.42
5:J:145:LEU:HD12	5:J:145:LEU:N	2.34	0.42
1:A:16:GLY:C	1:A:17:ARG:CD	2.93	0.42
1:A:260:HIS:HD2	1:A:271:THR:HG22	1.82	0.42
5:E:156:HIS:HB3	5:E:217:TYR:HB2	2.02	0.42
1:F:215:LEU:CD2	1:F:261:VAL:HG22	2.50	0.42
4:I:39:TYR:CD1	4:I:85:ALA:HB2	2.56	0.41
4:I:136:PHE:CE1	4:I:193:ILE:CG2	3.03	0.41
5:J:39:MET:HE1	5:J:89:VAL:HB	2.02	0.41
1:A:28:VAL:HG23	1:A:33:PHE:CD1	2.55	0.41
5:E:18:GLN:HB2	5:E:80:GLN:HG2	2.01	0.41
4:I:125:ASP:CG	4:I:128:SER:HB3	2.45	0.41
3:C:4:GLY:HA2	3:C:5:PRO:C	2.46	0.41
5:E:61:PRO:HG2	5:E:65:PHE:CG	2.56	0.41
1:F:219:ARG:HD2	1:F:219:ARG:O	2.20	0.41
2:G:7:ILE:HD13	2:G:82:VAL:HG21	2.03	0.41
5:J:52:ASN:OD1	5:J:69:MET:HE2	2.19	0.41
1:A:226:GLN:HG2	1:A:227:ASP:N	2.35	0.41
4:D:129:SER:O	4:D:131:LYS:N	2.53	0.41
5:E:35:TYR:HB3	5:E:43:LEU:HD22	2.02	0.41
1:F:268:LYS:HB2	1:F:268:LYS:NZ	2.35	0.41
5:E:185:LEU:N	5:E:185:LEU:HD12	2.36	0.41
1:F:51:TRP:CZ3	1:F:171:TYR:HB3	2.55	0.41
5:E:179:LEU:CD2	5:E:191:ALA:HB3	2.50	0.41
4:I:123:LEU:N	4:I:123:LEU:CD1	2.83	0.41
4:I:77:ARG:O	4:I:78:ASP:C	2.64	0.41
4:I:113:ILE:CD1	4:I:113:ILE:N	2.70	0.41
4:D:50:THR:CG2	4:D:56:LYS:HG3	2.51	0.41
5:E:198:VAL:HG11	5:E:210:PHE:HE2	1.85	0.41
1:F:226:GLN:O	1:F:227:ASP:HB3	2.20	0.41
2:G:27:VAL:HG23	2:G:30:PHE:HE1	1.86	0.41
2:G:84:HIS:CD2	2:G:86:THR:HG23	2.56	0.41
1:A:195:SER:O	1:A:196:ASP:HB3	2.20	0.41
1:A:232:GLU:O	1:A:233:THR:C	2.64	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:ARG:HG3	1:F:246:ALA:HB2	2.03	0.40
5:J:47:ILE:HG12	5:J:48:TYR:N	2.35	0.40
2:B:22:PHE:CZ	2:B:69:GLU:HG2	2.57	0.40
4:D:113:ILE:CD1	4:D:113:ILE:N	2.70	0.40
5:E:38:THR:OG1	5:E:41:ARG:HB3	2.22	0.40
4:I:191:SER:O	4:I:193:ILE:CD1	2.69	0.40
4:D:25:TYR:O	4:D:70:LYS:HB3	2.22	0.40
5:J:69:MET:HG2	5:J:75:SER:HB2	2.03	0.40
1:A:78:LEU:CD2	1:A:95:VAL:HG13	2.51	0.40
1:A:78:LEU:HD23	1:A:95:VAL:HG13	2.03	0.40
1:A:275:GLU:HB3	1:A:276:PRO:HD3	2.04	0.40
5:J:46:LEU:O	5:J:60:MET:HG2	2.22	0.40
1:A:145:HIS:HA	1:A:148:GLU:HG2	2.04	0.40
1:A:209:TYR:HA	1:A:210:PRO:O	2.22	0.40
4:D:161:LEU:HD13	4:D:161:LEU:C	2.47	0.40
5:E:15:MET:HE3	5:E:117:GLU:HG2	2.02	0.40
4:I:100:ILE:HD13	4:I:100:ILE:HA	1.95	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/276 (99%)	260 (95%)	14 (5%)	0	100	100
1	F	275/276 (100%)	255 (93%)	18 (6%)	2 (1%)	18	39
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	G	98/100 (98%)	91 (93%)	5 (5%)	2 (2%)	6	14
3	C	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	H	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
4	D	198/201 (98%)	185 (93%)	11 (6%)	2 (1%)	12	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	199/201 (99%)	187 (94%)	10 (5%)	2 (1%)	12	30
5	E	244/246 (99%)	228 (93%)	15 (6%)	1 (0%)	30	52
5	J	244/246 (99%)	236 (97%)	6 (2%)	2 (1%)	16	35
All	All	1646/1666 (99%)	1550 (94%)	85 (5%)	11 (1%)	18	39

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	130	ASP
1	F	227	ASP
5	J	64	ARG
5	E	85	ARG
4	I	151	SER
1	F	17	ARG
5	J	88	ALA
4	D	200	PRO
2	G	90	PRO
4	I	201	SER
2	G	14	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%)	225 (97%)	7 (3%)	36	64
1	F	233/232 (100%)	226 (97%)	7 (3%)	36	64
2	B	95/95 (100%)	93 (98%)	2 (2%)	47	73
2	G	95/95 (100%)	95 (100%)	0	100	100
3	C	5/5 (100%)	5 (100%)	0	100	100
3	H	5/5 (100%)	5 (100%)	0	100	100
4	D	181/182 (100%)	171 (94%)	10 (6%)	19	43
4	I	182/182 (100%)	169 (93%)	13 (7%)	13	32

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	216/216 (100%)	208 (96%)	8 (4%)	30	57
5	J	216/216 (100%)	211 (98%)	5 (2%)	44	71
All	All	1460/1460 (100%)	1408 (96%)	52 (4%)	31	58

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	17	ARG
1	A	31	THR
1	A	35	ARG
1	A	86	ASN
1	A	173	GLU
1	A	212	GLU
2	B	19	LYS
2	B	75	LYS
4	D	34	MET
4	D	41	ARG
4	D	48	MET
4	D	50	THR
4	D	60	ARG
4	D	65	VAL
4	D	99	LEU
4	D	109	VAL
4	D	113	ILE
4	D	181	ASP
5	E	9	ARG
5	E	60	MET
5	E	64	ARG
5	E	76	THR
5	E	80	GLN
5	E	141	GLN
5	E	222	ASN
5	E	244	ARG
1	F	12	VAL
1	F	35	ARG
1	F	218	GLN
1	F	219	ARG
1	F	226	GLN
1	F	258	THR
1	F	268	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	I	4	VAL
4	I	18	ILE
4	I	31	GLN
4	I	34	MET
4	I	65	VAL
4	I	99	LEU
4	I	109	VAL
4	I	113	ILE
4	I	123	LEU
4	I	133	VAL
4	I	152	ASP
4	I	181	ASP
4	I	193	ILE
5	J	39	MET
5	J	41	ARG
5	J	60	MET
5	J	141	GLN
5	J	195	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	86	ASN
1	A	93	HIS
1	A	141	GLN
1	A	180	GLN
1	A	188	HIS
1	A	218	GLN
1	A	226	GLN
1	A	260	HIS
2	B	13	HIS
2	B	51	HIS
4	D	31	GLN
4	D	38	GLN
4	D	144	ASN
4	D	171	ASN
4	D	178	ASN
4	D	186	ASN
4	D	189	ASN
5	E	17	GLN
5	E	29	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	E	37	GLN
5	E	50	ASN
5	E	80	GLN
5	E	103	ASN
5	E	121	ASN
5	E	182	GLN
5	E	186	ASN
5	E	215	GLN
5	E	222	ASN
1	F	70	HIS
1	F	86	ASN
1	F	87	GLN
1	F	93	HIS
1	F	180	GLN
1	F	188	HIS
1	F	197	HIS
1	F	218	GLN
1	F	226	GLN
1	F	255	GLN
2	G	13	HIS
2	G	24	ASN
2	G	84	HIS
4	I	22	ASN
4	I	31	GLN
4	I	171	ASN
4	I	178	ASN
4	I	189	ASN
4	I	190	ASN
5	J	29	HIS
5	J	51	ASN
5	J	103	ASN
5	J	121	ASN
5	J	141	GLN
5	J	182	GLN
5	J	186	ASN

### 5.3.3 RNA

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	SO4	A	277	-	4,4,4	0.28	0	6,6,6	0.13	0
6	SO4	F	277	-	4,4,4	0.28	0	6,6,6	0.05	0
6	SO4	D	203	-	4,4,4	0.30	0	6,6,6	0.11	0
7	GOL	J	247	-	5,5,5	0.71	0	5,5,5	0.36	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
7	GOL	J	247	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	247	GOL	O1-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
7	J	247	GOL	C1-C2-C3-O3
7	J	247	GOL	O1-C1-C2-O2
7	J	247	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	277	SO4	1	0
6	F	277	SO4	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	276/276 (100%)	-1.29	0 100 100	25, 56, 98, 118	0
1	F	276/276 (100%)	-1.02	0 100 100	28, 69, 141, 173	1 (0%)
2	B	100/100 (100%)	-1.22	0 100 100	30, 55, 98, 119	0
2	G	100/100 (100%)	-1.10	0 100 100	35, 62, 99, 128	0
3	C	10/10 (100%)	-1.49	0 100 100	31, 32, 38, 40	0
3	H	10/10 (100%)	-1.34	0 100 100	30, 35, 44, 47	0
4	D	200/201 (99%)	-1.26	0 100 100	28, 53, 97, 131	0
4	I	201/201 (100%)	-1.31	0 100 100	26, 49, 88, 111	0
5	E	246/246 (100%)	-1.18	0 100 100	26, 55, 103, 139	0
5	J	246/246 (100%)	-1.41	0 100 100	25, 45, 89, 108	0
All	All	1665/1666 (99%)	-1.23	0 100 100	25, 55, 106, 173	1 (0%)

There are no RSRZ outliers to report.

### 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 oligosaccharides 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	SO4	A	277	5/5	0.91	0.09	99,100,100,100	0
6	SO4	F	277	5/5	0.96	0.07	100,100,100,100	0
6	SO4	D	203	5/5	0.98	0.07	100,100,100,100	0
7	GOL	J	247	6/6	0.98	0.08	42,69,71,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.