



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:32 am GMT

PDB ID : 5C09  
Title : HLA class I histocompatibility antigen  
Authors : Rizkallah, P.J.; Bulek, A.M.; Cole, D.K.; Sewell, A.K.  
Deposited on : 2015-06-12  
Resolution : 2.48 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

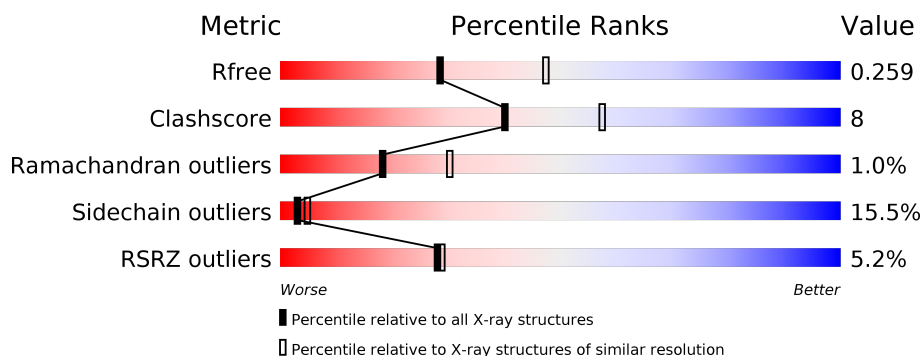
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 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))
$R_{free}$	100719	4719 (2.50-2.46)
Clashscore	112137	5483 (2.50-2.46)
Ramachandran outliers	110173	5388 (2.50-2.46)
Sidechain outliers	110143	5390 (2.50-2.46)
RSRZ outliers	101464	4754 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
1	F	276	<div> <div>3%</div> <div>74%</div> <div>22%</div> <div>.</div> </div>
2	B	100	<div> <div>%</div> <div>71%</div> <div>23%</div> <div>6%</div> </div>
2	G	100	<div> <div>2%</div> <div>74%</div> <div>25%</div> <div>.</div> </div>
3	C	10	<div> <div>80%</div> <div>20%</div> </div>
3	H	10	<div> <div>90%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	200	
4	I	200	
5	E	246	
5	J	246	

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	SO4	A	303	-	-	-	X
6	SO4	D	301	-	-	-	X
6	SO4	F	301	-	-	-	X
6	SO4	I	301	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13529 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
			77	52	10	15			
3	H	10	Total	C	N	O	0	0	0
			77	52	10	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	197	Total	C	N	O	S	0	0	0
			1557	975	256	316	10			

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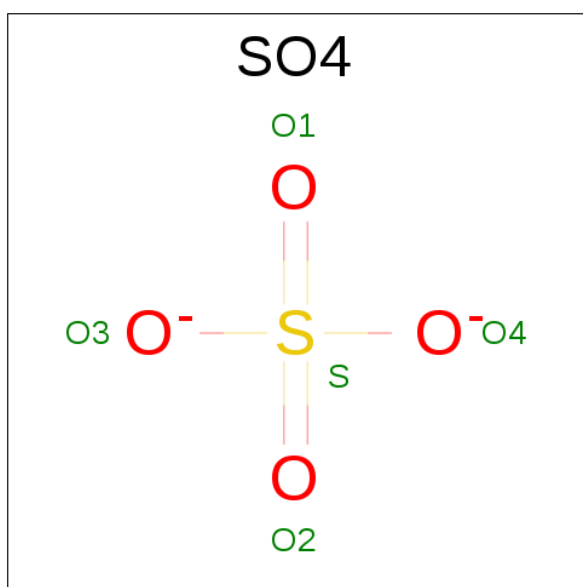
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	200	Total	C	N	O	S	0	0	0
			1577	988	259	320	10			

- 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	246	Total	C	N	O	S	0	0	0
			1974	1249	341	374	10			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		

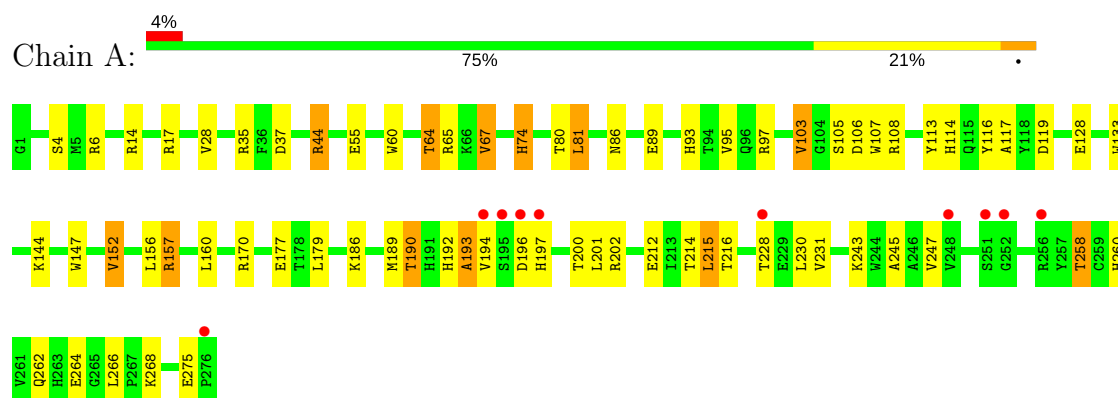
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	15	Total	O	0	0
			15	15		
7	B	10	Total	O	0	0
			10	10		
7	C	1	Total	O	0	0
			1	1		
7	D	7	Total	O	0	0
			7	7		
7	E	10	Total	O	0	0
			10	10		
7	F	16	Total	O	0	0
			16	16		
7	G	6	Total	O	0	0
			6	6		
7	H	1	Total	O	0	0
			1	1		
7	I	4	Total	O	0	0
			4	4		
7	J	14	Total	O	0	0
			14	14		

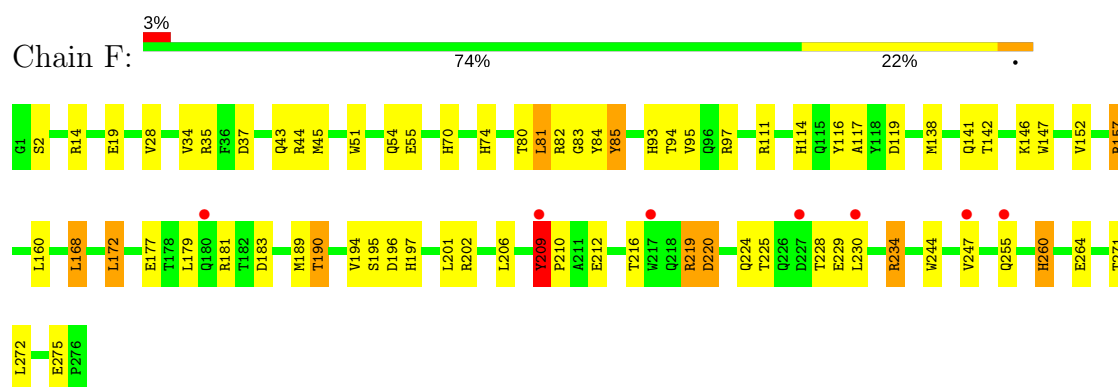
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

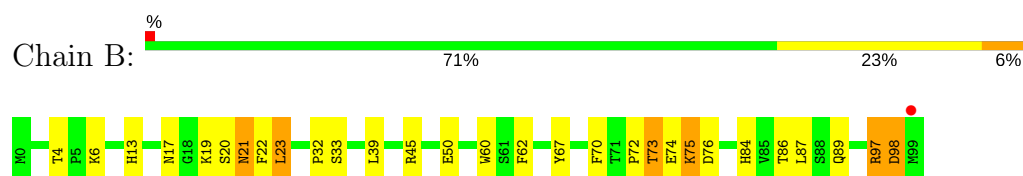
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



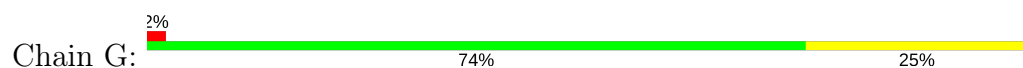
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

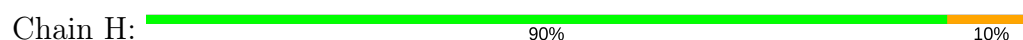




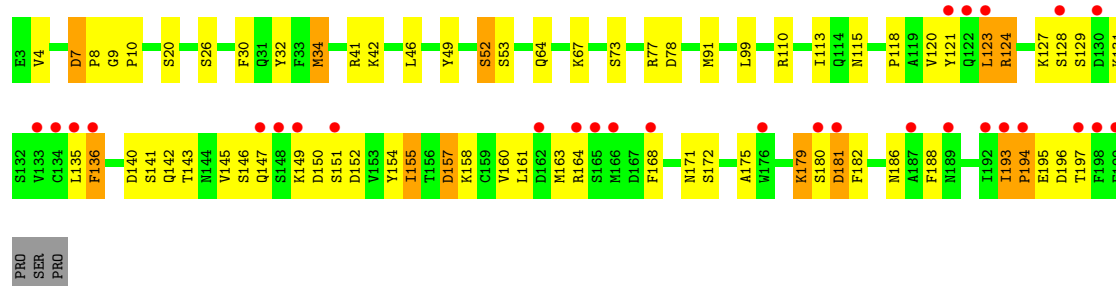
- Molecule 3: Marker peptide



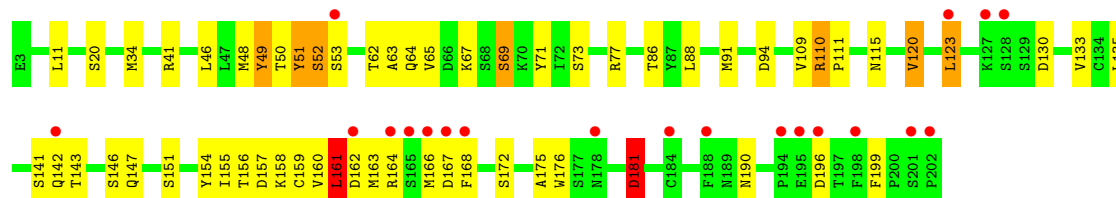
- Molecule 3: Marker peptide



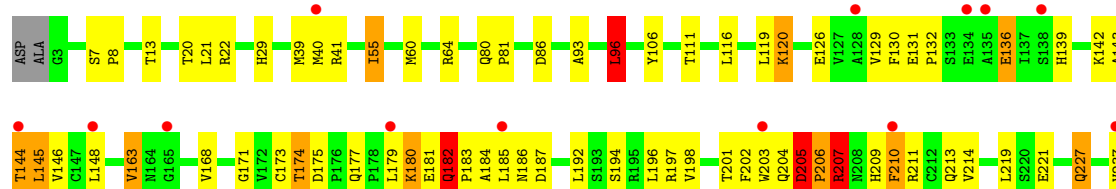
- Molecule 4: 1E6 TCR Alpha Chain



- Molecule 4: 1E6 TCR Alpha Chain



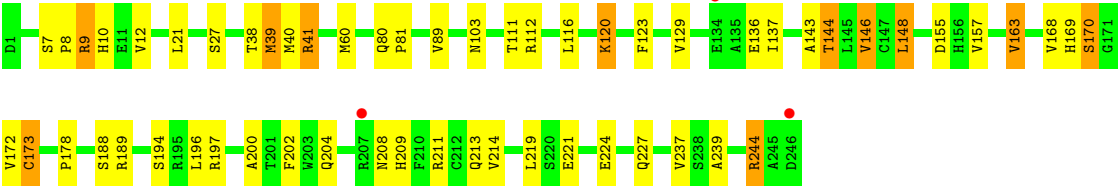
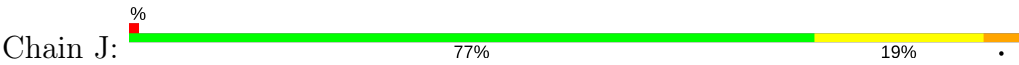
- Molecule 5: 1E6 TCR Beta Chain







● Molecule 5: 1E6 TCR Beta Chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.83Å 100.07Å 122.44Å 96.91° 98.31° 96.52°	Depositor
Resolution (Å)	98.46 – 2.48 98.46 – 2.47	Depositor EDS
% Data completeness (in resolution range)	98.2 (98.46-2.48) 93.7 (98.46-2.47)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.205 , 0.259 0.208 , 0.259	Depositor DCC
$R_{free}$ test set	3581 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.3	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 38.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.71	0/2320	0.90	4/3149 (0.1%)
1	F	0.65	0/2320	0.91	6/3149 (0.2%)
2	B	0.75	0/860	0.91	1/1162 (0.1%)
2	G	0.72	0/860	0.85	1/1162 (0.1%)
3	C	0.83	0/80	0.71	0/108
3	H	0.88	0/80	0.91	0/108
4	D	0.64	0/1592	0.84	0/2154
4	I	0.65	0/1614	0.86	2/2186 (0.1%)
5	E	0.68	0/2016	0.86	2/2741 (0.1%)
5	J	0.72	0/2029	0.86	2/2759 (0.1%)
All	All	0.69	0/13771	0.87	18/18678 (0.1%)

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	1
4	D	0	1
4	I	0	1
5	E	0	4
5	J	0	1
All	All	0	8

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	161	LEU	CA-CB-CG	8.10	133.93	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ARG	CG-CD-NE	-7.39	96.28	111.80
2	B	97	ARG	NE-CZ-NH1	-7.19	116.71	120.30
1	F	85	TYR	CB-CA-C	6.53	123.45	110.40
5	E	96	LEU	CA-CB-CG	6.39	130.00	115.30
1	F	85	TYR	N-CA-C	-6.28	94.05	111.00
1	A	67	VAL	CB-CA-C	-6.21	99.61	111.40
1	F	37	ASP	CB-CG-OD1	5.78	123.50	118.30
1	F	209	TYR	C-N-CD	5.74	140.45	128.40
1	A	37	ASP	CB-CG-OD1	5.53	123.27	118.30
5	J	173	CYS	CA-CB-SG	5.44	123.79	114.00
1	A	157	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	G	97	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	F	234	ARG	NE-CZ-NH1	5.21	122.90	120.30
4	I	110	ARG	NE-CZ-NH2	-5.17	117.72	120.30
5	J	60	MET	CG-SD-CE	-5.14	91.98	100.20
1	F	157	ARG	NE-CZ-NH1	5.04	122.82	120.30
5	E	60	MET	CG-SD-CE	-5.02	92.17	100.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	ALA	Peptide
4	D	8	PRO	Peptide
5	E	181	GLU	Peptide
5	E	182	GLN	Peptide
5	E	205	ASP	Peptide
5	E	207	ARG	Peptide
4	I	151	SER	Peptide
5	J	39	MET	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2254	0	2103	35	0
1	F	2254	0	2103	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	837	0	803	23	0
2	G	837	0	803	13	0
3	C	77	0	73	1	0
3	H	77	0	73	1	0
4	D	1557	0	1471	42	0
4	I	1577	0	1488	23	0
5	E	1961	0	1875	42	0
5	J	1974	0	1887	33	0
6	A	15	0	0	0	0
6	D	5	0	0	0	0
6	F	10	0	0	1	0
6	I	5	0	0	0	0
6	J	5	0	0	0	0
7	A	15	0	0	1	0
7	B	10	0	0	1	0
7	C	1	0	0	0	0
7	D	7	0	0	0	0
7	E	10	0	0	1	0
7	F	16	0	0	0	0
7	G	6	0	0	0	0
7	H	1	0	0	0	0
7	I	4	0	0	0	0
7	J	14	0	0	0	0
All	All	13529	0	12679	216	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 8.

All (216) 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:180:LYS:HB2	5:E:182:GLN:HG3	1.54	0.89
4:D:161:LEU:HD21	5:E:171:GLY:O	1.82	0.79
1:A:60:TRP:O	1:A:64:THR:HG23	1.85	0.77
1:F:138:MET:HA	1:F:141:GLN:HG3	1.69	0.75
5:E:183:PRO:O	5:E:185:LEU:N	2.20	0.74
5:E:185:LEU:O	5:E:187:ASP:N	2.20	0.74
1:A:86:ASN:ND2	7:A:401:HOH:O	2.20	0.74
4:D:193:ILE:HB	4:D:194:PRO:HD3	1.71	0.72
2:B:73:THR:HG22	2:B:76:ASP:H	1.55	0.72
4:D:136:PHE:CZ	4:D:188:PHE:HE1	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:123:LEU:HD21	5:E:131:GLU:O	1.90	0.71
4:D:32:TYR:HB3	4:D:34:MET:HE1	1.71	0.70
2:B:13:HIS:H	2:B:21:ASN:HD21	1.39	0.70
4:I:62:THR:OG1	4:I:77:ARG:NH2	2.22	0.70
5:E:180:LYS:HB2	5:E:182:GLN:CG	2.21	0.70
4:D:113:ILE:HG12	4:D:140:ASP:HA	1.74	0.68
5:E:29:HIS:HA	5:E:96:LEU:HD13	1.76	0.68
4:D:4:VAL:HG22	4:D:91:MET:CE	2.24	0.67
5:E:29:HIS:HA	5:E:96:LEU:CD1	2.25	0.67
5:E:132:PRO:HG3	5:E:144:THR:O	1.94	0.66
5:E:163:VAL:HA	5:E:209:HIS:O	1.96	0.66
1:F:219:ARG:O	1:F:220:ASP:OD1	2.14	0.65
2:B:21:ASN:HD22	2:B:22:PHE:H	1.45	0.65
4:D:121:TYR:CE2	5:E:136:GLU:HG3	2.32	0.64
5:J:155:ASP:OD1	5:J:178:PRO:HG3	1.97	0.64
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.81	0.64
1:A:103:VAL:HG13	1:A:107:TRP:HA	1.79	0.63
4:D:118:PRO:O	4:D:196:ASP:HB3	1.97	0.63
4:D:123:LEU:CD2	5:E:131:GLU:O	2.45	0.63
1:A:65:ARG:HG3	5:E:55:ILE:CD1	2.29	0.63
5:J:169:HIS:O	5:J:172:VAL:HG22	1.99	0.63
1:F:93:HIS:HD2	1:F:119:ASP:OD2	1.81	0.62
5:J:211:ARG:NH2	5:J:213:GLN:HE21	1.98	0.62
5:J:38:THR:O	5:J:40:MET:O	2.18	0.61
4:D:4:VAL:HG22	4:D:91:MET:HE1	1.81	0.61
5:J:163:VAL:HA	5:J:209:HIS:O	2.00	0.61
2:B:4:THR:HG22	2:B:86:THR:CB	2.32	0.60
2:B:17:ASN:OD1	2:B:97:ARG:NH1	2.30	0.59
1:F:234:ARG:HD3	2:G:10:TYR:CZ	2.37	0.59
1:F:190:THR:HG22	1:F:202:ARG:HB3	1.85	0.58
4:D:30:PHE:CE2	4:D:91:MET:HE3	2.39	0.58
2:B:89:GLN:NE2	7:B:101:HOH:O	2.37	0.57
1:A:215:LEU:HD22	1:A:243:LYS:HD3	1.86	0.57
5:J:144:THR:HG23	5:J:197:ARG:HG2	1.87	0.57
4:D:157:ASP:OD1	4:D:157:ASP:N	2.35	0.57
1:A:89:GLU:OE1	5:J:27:SER:OG	2.23	0.57
1:A:190:THR:HG22	1:A:202:ARG:HB3	1.86	0.56
4:D:128:SER:OG	4:D:129:SER:N	2.37	0.56
1:F:260:HIS:CE1	1:F:271:THR:HG22	2.39	0.56
1:A:6:ARG:NH2	1:A:113:TYR:OH	2.36	0.56
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:161:LEU:HB3	5:J:173:CYS:HB2	1.88	0.56
5:E:201:THR:HA	5:E:204:GLN:NE2	2.21	0.56
4:I:166:MET:O	4:I:168:PHE:N	2.39	0.55
4:D:180:SER:O	4:D:182:PHE:N	2.38	0.55
2:B:4:THR:HG22	2:B:86:THR:HB	1.88	0.55
5:E:21:LEU:HD22	5:E:111:THR:HG21	1.89	0.55
1:A:97:ARG:HH11	1:A:114:HIS:HE1	1.54	0.55
4:D:161:LEU:CD2	5:E:171:GLY:O	2.52	0.55
1:A:60:TRP:O	1:A:64:THR:CG2	2.55	0.54
5:E:126:GLU:HA	5:E:126:GLU:OE1	2.06	0.54
1:F:183:ASP:H	1:F:209:TYR:HB2	1.72	0.54
1:F:196:ASP:O	1:F:197:HIS:CG	2.61	0.54
1:F:196:ASP:O	1:F:197:HIS:CD2	2.60	0.54
5:J:129:VAL:HG23	5:J:239:ALA:HB3	1.89	0.54
1:F:209:TYR:HB3	1:F:210:PRO:CD	2.37	0.54
4:D:195:GLU:N	4:D:195:GLU:OE1	2.38	0.54
5:E:139:HIS:CE1	7:E:306:HOH:O	2.61	0.54
4:I:120:VAL:HG11	4:I:199:PHE:CE2	2.42	0.54
1:A:81:LEU:HD13	3:C:10:ILE:HG21	1.90	0.54
1:F:84:TYR:C	1:F:85:TYR:O	2.42	0.54
4:I:120:VAL:HG11	4:I:199:PHE:CZ	2.43	0.53
4:D:4:VAL:CG2	4:D:91:MET:HE2	2.39	0.53
1:A:74:HIS:HE1	1:A:97:ARG:HE	1.55	0.53
4:D:136:PHE:N	4:D:136:PHE:CD1	2.76	0.53
5:J:211:ARG:HH21	5:J:213:GLN:HE21	1.57	0.53
5:E:145:LEU:HD23	5:E:196:LEU:O	2.09	0.52
2:B:19:LYS:O	2:B:72:PRO:HD2	2.09	0.52
1:F:97:ARG:HH11	1:F:114:HIS:HE1	1.56	0.52
2:G:4:THR:CG2	2:G:86:THR:OG1	2.57	0.52
1:A:230:LEU:HD23	1:A:245:ALA:HB2	1.91	0.52
2:G:32:PRO:O	2:G:84:HIS:HE1	1.93	0.52
4:D:179:LYS:HD3	4:D:179:LYS:N	2.25	0.52
2:B:21:ASN:ND2	2:B:22:PHE:H	2.07	0.52
4:D:120:VAL:HG22	4:D:136:PHE:HB3	1.92	0.52
4:D:140:ASP:OD2	4:D:142:GLN:HB3	2.10	0.52
5:E:143:ALA:O	5:E:197:ARG:HA	2.10	0.52
5:E:55:ILE:HD12	5:E:55:ILE:C	2.30	0.52
5:J:136:GLU:OE2	5:J:197:ARG:NH2	2.43	0.52
2:G:19:LYS:O	2:G:72:PRO:HD2	2.10	0.51
4:D:160:VAL:HG22	4:D:171:ASN:ND2	2.26	0.51
5:E:204:GLN:O	5:E:244:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:LEU:HD22	1:F:172:LEU:HD22	1.93	0.51
5:J:137:ILE:HG23	5:J:200:ALA:HB1	1.93	0.51
4:I:176:TRP:CH2	5:J:148:LEU:HD21	2.46	0.51
5:J:157:VAL:HG13	5:J:214:VAL:HG13	1.93	0.50
2:G:84:HIS:HD2	2:G:86:THR:OG1	1.94	0.50
2:B:4:THR:HG22	2:B:86:THR:OG1	2.11	0.50
1:F:234:ARG:HD3	2:G:10:TYR:CE1	2.46	0.50
5:J:120:LYS:HE2	5:J:227:GLN:NE2	2.27	0.50
4:D:30:PHE:CD2	4:D:91:MET:HE3	2.46	0.50
1:F:209:TYR:O	1:F:210:PRO:C	2.47	0.50
5:J:40:MET:SD	5:J:41:ARG:NE	2.84	0.50
2:B:32:PRO:O	2:B:84:HIS:HE1	1.93	0.49
1:A:128:GLU:OE1	1:A:128:GLU:N	2.45	0.49
2:B:84:HIS:HD2	2:B:86:THR:OG1	1.93	0.49
5:J:9:ARG:HG2	5:J:10:HIS:ND1	2.27	0.49
4:D:110:ARG:HB3	4:D:141:SER:HB3	1.95	0.48
1:A:55:GLU:OE1	1:A:170:ARG:NH2	2.46	0.48
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.47	0.48
5:J:143:ALA:O	5:J:197:ARG:HA	2.12	0.48
1:F:209:TYR:HB3	1:F:210:PRO:HD3	1.96	0.48
1:F:83:GLY:O	1:F:85:TYR:O	2.31	0.48
1:A:258:THR:CG2	1:A:260:HIS:CE1	2.97	0.48
4:D:124:ARG:NH2	4:D:129:SER:OG	2.48	0.47
1:A:97:ARG:HH11	1:A:114:HIS:CE1	2.31	0.47
1:A:202:ARG:NH1	2:B:98:ASP:O	2.48	0.47
5:E:132:PRO:HD2	5:E:203:TRP:CZ2	2.50	0.47
1:A:147:TRP:HB3	1:A:152:VAL:HG13	1.97	0.47
2:G:23:LEU:O	2:G:67:TYR:HA	2.14	0.47
4:I:49:TYR:HH	4:I:51:TYR:HE2	1.61	0.47
2:B:23:LEU:O	2:B:67:TYR:HA	2.14	0.47
2:B:89:GLN:HE21	5:J:211:ARG:NH1	2.13	0.46
1:F:168:LEU:O	1:F:172:LEU:HD22	2.15	0.46
1:A:147:TRP:O	1:A:152:VAL:HG13	2.15	0.46
5:E:55:ILE:HD12	5:E:55:ILE:O	2.14	0.46
1:F:81:LEU:HD13	3:H:10:ILE:HG21	1.97	0.46
4:I:110:ARG:HB3	4:I:141:SER:HB3	1.97	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CZ2	2.51	0.46
4:D:196:ASP:OD1	4:D:197:THR:N	2.49	0.46
1:F:244:TRP:NE1	2:G:99:MET:HG2	2.30	0.46
5:J:204:GLN:HA	5:J:244:ARG:O	2.16	0.46
1:A:193:ALA:HB1	1:A:194:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:145:LEU:HD11	5:E:210:PHE:CE1	2.51	0.46
4:I:164:ARG:HB2	5:J:170:SER:HB3	1.98	0.46
4:D:168:PHE:CE1	5:E:197:ARG:NH2	2.84	0.46
2:G:4:THR:HG23	2:G:86:THR:OG1	2.16	0.46
4:D:9:GLY:O	4:D:10:PRO:C	2.52	0.45
4:D:136:PHE:CZ	4:D:188:PHE:CE1	2.96	0.45
1:F:260:HIS:CE1	1:F:271:THR:CG2	2.99	0.45
1:F:97:ARG:HH11	1:F:114:HIS:CE1	2.34	0.45
5:J:202:PHE:O	5:J:208:ASN:ND2	2.42	0.45
4:D:4:VAL:HG22	4:D:91:MET:HE2	1.94	0.45
1:A:192:HIS:HB2	1:A:200:THR:CG2	2.47	0.45
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.51	0.45
4:I:46:LEU:HD22	5:J:103:ASN:O	2.17	0.45
5:J:144:THR:HG23	5:J:197:ARG:CG	2.45	0.45
1:A:214:THR:OG1	1:A:262:GLN:HB2	2.16	0.45
2:G:33:SER:HB3	2:G:62:PHE:CE2	2.52	0.45
5:E:211:ARG:NH2	5:E:213:GLN:OE1	2.50	0.45
1:A:189:MET:CE	1:A:201:LEU:HD22	2.47	0.45
4:D:147:GLN:NE2	4:D:155:ILE:O	2.50	0.44
1:F:189:MET:CE	1:F:201:LEU:HD22	2.47	0.44
5:E:93:ALA:HA	5:E:106:TYR:O	2.18	0.44
1:F:229:GLU:HG3	1:F:229:GLU:O	2.16	0.44
4:I:161:LEU:CB	5:J:173:CYS:HB2	2.47	0.44
5:E:174:THR:HA	5:E:194:SER:HA	1.99	0.44
4:I:181:ASP:OD1	4:I:181:ASP:C	2.56	0.44
1:A:106:ASP:OD1	1:A:108:ARG:HG2	2.17	0.44
4:D:113:ILE:HD12	4:D:113:ILE:O	2.18	0.44
4:D:145:VAL:HG22	4:D:155:ILE:HD11	2.00	0.44
5:E:64:ARG:NH1	5:E:86:ASP:OD2	2.51	0.44
1:F:196:ASP:OD1	1:F:196:ASP:N	2.49	0.44
5:J:8:PRO:O	5:J:111:THR:HG23	2.18	0.44
5:J:157:VAL:HG13	5:J:214:VAL:CG1	2.47	0.44
1:A:65:ARG:HG3	5:E:55:ILE:HD12	1.97	0.43
4:D:193:ILE:HB	4:D:194:PRO:CD	2.45	0.43
4:D:30:PHE:CE2	4:D:91:MET:CE	3.01	0.43
4:D:7:ASP:OD1	4:D:7:ASP:N	2.46	0.43
5:E:22:ARG:NE	6:F:302:SO4:O2	2.47	0.43
1:F:95:VAL:HG11	1:F:116:TYR:OH	2.18	0.43
1:A:95:VAL:HG11	1:A:116:TYR:OH	2.18	0.43
4:D:154:TYR:O	4:D:175:ALA:HA	2.19	0.43
4:I:69:SER:OG	4:I:71:TYR:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:THR:HG23	2:B:75:LYS:HE3	2.00	0.43
4:D:123:LEU:HD23	5:E:130:PHE:HB3	2.00	0.43
4:I:50:THR:OG1	4:I:65:VAL:HG21	2.18	0.43
4:D:136:PHE:CE2	4:D:188:PHE:HE1	2.35	0.43
4:I:111:PRO:HG3	4:I:160:VAL:HG21	2.01	0.43
2:B:73:THR:HG23	2:B:74:GLU:N	2.33	0.42
2:B:21:ASN:HD22	2:B:22:PHE:N	2.14	0.42
1:F:51:TRP:O	1:F:54:GLN:HG2	2.19	0.42
4:I:123:LEU:HD22	5:J:146:VAL:HG13	2.01	0.42
5:J:173:CYS:O	5:J:194:SER:HA	2.19	0.42
5:E:8:PRO:O	5:E:111:THR:HG23	2.20	0.42
1:A:106:ASP:CG	1:A:108:ARG:HG2	2.39	0.42
5:E:182:GLN:HB2	5:E:183:PRO:O	2.20	0.42
4:I:190:ASN:N	4:I:190:ASN:HD22	2.17	0.42
5:E:80:GLN:HA	5:E:81:PRO:HA	1.92	0.41
1:A:133:TRP:HB2	1:A:144:LYS:HE2	2.03	0.41
5:E:182:GLN:HE21	5:E:182:GLN:H	1.66	0.41
2:B:73:THR:CG2	2:B:76:ASP:H	2.29	0.41
5:E:120:LYS:HG2	5:E:227:GLN:OE1	2.21	0.41
5:E:145:LEU:CD2	5:E:196:LEU:O	2.68	0.41
1:F:147:TRP:O	1:F:152:VAL:HG23	2.20	0.41
2:G:98:ASP:O	2:G:99:MET:CB	2.68	0.41
5:E:206:PRO:HB2	5:E:207:ARG:H	1.71	0.41
1:A:189:MET:HE1	1:A:201:LEU:HD22	2.02	0.41
4:I:48:MET:HG2	4:I:63:ALA:HB2	2.03	0.41
4:I:155:ILE:HG12	4:I:175:ALA:CB	2.50	0.41
4:I:120:VAL:CG1	4:I:199:PHE:CE2	3.04	0.41
4:D:77:ARG:O	4:D:78:ASP:C	2.59	0.41
4:I:154:TYR:O	4:I:175:ALA:HA	2.20	0.41
4:I:133:VAL:HG23	4:I:176:TRP:HB3	2.02	0.41
4:D:146:SER:O	4:D:155:ILE:HD13	2.20	0.41
2:G:4:THR:HG22	2:G:86:THR:OG1	2.20	0.41
5:J:123:PHE:CD1	5:J:189:ARG:HD3	2.56	0.41
2:B:89:GLN:NE2	5:J:211:ARG:NH1	2.69	0.41
1:A:28:VAL:HG11	1:A:179:LEU:HD13	2.03	0.41
1:F:219:ARG:HG3	1:F:219:ARG:O	2.17	0.40
5:J:80:GLN:HA	5:J:81:PRO:HA	1.89	0.40
1:F:70:HIS:O	1:F:74:HIS:HD2	2.03	0.40
5:J:89:VAL:HG22	5:J:112:ARG:HG3	2.02	0.40
1:A:65:ARG:CG	5:E:55:ILE:CD1	2.99	0.40
5:E:227:GLN:HE21	5:E:227:GLN:HB3	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:156:THR:HG22	4:I:157:ASP:O	2.21	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%)	266 (97%)	7 (3%)	1 (0%)	38	57
1	F	274/276 (99%)	263 (96%)	9 (3%)	2 (1%)	25	41
2	B	98/100 (98%)	95 (97%)	2 (2%)	1 (1%)	18	30
2	G	98/100 (98%)	96 (98%)	2 (2%)	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	195/200 (98%)	177 (91%)	14 (7%)	4 (2%)	8	12
4	I	198/200 (99%)	177 (89%)	17 (9%)	4 (2%)	9	13
5	E	242/246 (98%)	228 (94%)	10 (4%)	4 (2%)	11	17
5	J	244/246 (99%)	238 (98%)	6 (2%)	0	100	100
All	All	1639/1664 (98%)	1555 (95%)	68 (4%)	16 (1%)	18	30

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	52	SER
4	D	181	ASP
5	E	184	ALA
4	I	167	ASP
1	A	196	ASP
5	E	206	PRO

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Mol	Chain	Res	Type
5	E	186	ASN
1	F	209	TYR
4	D	193	ILE
5	E	205	ASP
4	I	52	SER
4	I	181	ASP
2	B	98	ASP
1	F	264	GLU
4	I	41	ARG
4	D	194	PRO

### 5.3.2 Protein sidechains ⓘ

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%)	201 (87%)	31 (13%)	4	7
1	F	232/232 (100%)	190 (82%)	42 (18%)	2	3
2	B	95/95 (100%)	84 (88%)	11 (12%)	6	11
2	G	95/95 (100%)	83 (87%)	12 (13%)	5	9
3	C	8/8 (100%)	7 (88%)	1 (12%)	5	9
3	H	8/8 (100%)	7 (88%)	1 (12%)	5	9
4	D	178/181 (98%)	143 (80%)	35 (20%)	1	2
4	I	181/181 (100%)	148 (82%)	33 (18%)	2	3
5	E	215/216 (100%)	176 (82%)	39 (18%)	2	3
5	J	216/216 (100%)	195 (90%)	21 (10%)	9	16
All	All	1460/1464 (100%)	1234 (84%)	226 (16%)	3	5

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	14	ARG
1	A	17	ARG

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Mol	Chain	Res	Type
1	A	35	ARG
1	A	44	ARG
1	A	64	THR
1	A	67	VAL
1	A	74	HIS
1	A	80	THR
1	A	81	LEU
1	A	103	VAL
1	A	105	SER
1	A	152	VAL
1	A	156	LEU
1	A	157	ARG
1	A	160	LEU
1	A	177	GLU
1	A	186	LYS
1	A	190	THR
1	A	197	HIS
1	A	212	GLU
1	A	215	LEU
1	A	216	THR
1	A	228	THR
1	A	231	VAL
1	A	247	VAL
1	A	258	THR
1	A	264	GLU
1	A	266	LEU
1	A	268	LYS
1	A	275	GLU
2	B	6	LYS
2	B	20	SER
2	B	21	ASN
2	B	23	LEU
2	B	39	LEU
2	B	45	ARG
2	B	50	GLU
2	B	70	PHE
2	B	73	THR
2	B	75	LYS
2	B	87	LEU
3	C	9	THR
4	D	7	ASP
4	D	20	SER

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Mol	Chain	Res	Type
4	D	26	SER
4	D	34	MET
4	D	41	ARG
4	D	42	LYS
4	D	46	LEU
4	D	49	TYR
4	D	52	SER
4	D	53	SER
4	D	64	GLN
4	D	67	LYS
4	D	73	SER
4	D	99	LEU
4	D	115	ASN
4	D	123	LEU
4	D	124	ARG
4	D	127	LYS
4	D	131	LYS
4	D	135	LEU
4	D	136	PHE
4	D	143	THR
4	D	149	LYS
4	D	150	ASP
4	D	151	SER
4	D	152	ASP
4	D	155	ILE
4	D	157	ASP
4	D	158	LYS
4	D	163	MET
4	D	164	ARG
4	D	172	SER
4	D	179	LYS
4	D	181	ASP
4	D	186	ASN
5	E	7	SER
5	E	13	THR
5	E	20	THR
5	E	39	MET
5	E	40	MET
5	E	41	ARG
5	E	55	ILE
5	E	96	LEU
5	E	116	LEU

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Mol	Chain	Res	Type
5	E	119	LEU
5	E	120	LYS
5	E	129	VAL
5	E	136	GLU
5	E	142	LYS
5	E	144	THR
5	E	145	LEU
5	E	146	VAL
5	E	148	LEU
5	E	163	VAL
5	E	168	VAL
5	E	173	CYS
5	E	174	THR
5	E	175	ASP
5	E	177	GLN
5	E	179	LEU
5	E	180	LYS
5	E	182	GLN
5	E	192	LEU
5	E	198	VAL
5	E	202	PHE
5	E	205	ASP
5	E	207	ARG
5	E	210	PHE
5	E	214	VAL
5	E	219	LEU
5	E	221	GLU
5	E	227	GLN
5	E	237	VAL
5	E	244	ARG
1	F	2	SER
1	F	14	ARG
1	F	19	GLU
1	F	28	VAL
1	F	34	VAL
1	F	35	ARG
1	F	43	GLN
1	F	44	ARG
1	F	45	MET
1	F	55	GLU
1	F	80	THR
1	F	81	LEU

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Mol	Chain	Res	Type
1	F	82	ARG
1	F	94	THR
1	F	111	ARG
1	F	142	THR
1	F	146	LYS
1	F	157	ARG
1	F	160	LEU
1	F	168	LEU
1	F	172	LEU
1	F	177	GLU
1	F	179	LEU
1	F	181	ARG
1	F	190	THR
1	F	194	VAL
1	F	195	SER
1	F	206	LEU
1	F	209	TYR
1	F	212	GLU
1	F	216	THR
1	F	219	ARG
1	F	220	ASP
1	F	224	GLN
1	F	225	THR
1	F	228	THR
1	F	230	LEU
1	F	247	VAL
1	F	255	GLN
1	F	260	HIS
1	F	272	LEU
1	F	275	GLU
2	G	1	ILE
2	G	4	THR
2	G	20	SER
2	G	34	ASP
2	G	41	LYS
2	G	45	ARG
2	G	47	GLU
2	G	50	GLU
2	G	57	SER
2	G	70	PHE
2	G	71	THR
2	G	85	VAL

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Mol	Chain	Res	Type
3	H	10	ILE
4	I	11	LEU
4	I	20	SER
4	I	34	MET
4	I	49	TYR
4	I	51	TYR
4	I	52	SER
4	I	53	SER
4	I	64	GLN
4	I	67	LYS
4	I	69	SER
4	I	73	SER
4	I	86	THR
4	I	88	LEU
4	I	91	MET
4	I	94	ASP
4	I	109	VAL
4	I	115	ASN
4	I	120	VAL
4	I	123	LEU
4	I	130	ASP
4	I	135	LEU
4	I	142	GLN
4	I	143	THR
4	I	146	SER
4	I	147	GLN
4	I	158	LYS
4	I	159	CYS
4	I	161	LEU
4	I	162	ASP
4	I	163	MET
4	I	172	SER
4	I	181	ASP
4	I	196	ASP
5	J	7	SER
5	J	9	ARG
5	J	12	VAL
5	J	21	LEU
5	J	39	MET
5	J	41	ARG
5	J	116	LEU
5	J	120	LYS

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Mol	Chain	Res	Type
5	J	144	THR
5	J	146	VAL
5	J	148	LEU
5	J	163	VAL
5	J	168	VAL
5	J	170	SER
5	J	188	SER
5	J	196	LEU
5	J	219	LEU
5	J	221	GLU
5	J	224	GLU
5	J	237	VAL
5	J	244	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	54	GLN
1	A	70	HIS
1	A	74	HIS
1	A	93	HIS
1	A	114	HIS
1	A	141	GLN
1	A	174	ASN
1	A	260	HIS
2	B	21	ASN
2	B	84	HIS
2	B	89	GLN
4	D	64	GLN
4	D	171	ASN
4	D	186	ASN
5	E	10	HIS
1	F	3	HIS
1	F	54	GLN
1	F	72	GLN
1	F	87	GLN
1	F	93	HIS
1	F	114	HIS
1	F	115	GLN
1	F	260	HIS
2	G	8	GLN

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Mol	Chain	Res	Type
2	G	84	HIS
4	I	64	GLN
4	I	171	ASN
4	I	190	ASN
5	J	141	GLN
5	J	204	GLN
5	J	213	GLN
5	J	227	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

8 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	301	-	4,4,4	0.53	0	6,6,6	0.61	0
6	SO4	A	302	-	4,4,4	0.49	0	6,6,6	0.22	0
6	SO4	A	303	-	4,4,4	0.41	0	6,6,6	0.32	0
6	SO4	D	301	-	4,4,4	0.54	0	6,6,6	0.20	0
6	SO4	F	301	-	4,4,4	0.45	0	6,6,6	0.79	0
6	SO4	F	302	-	4,4,4	0.53	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	I	301	-	4,4,4	0.46	0	6,6,6	0.15	0
6	SO4	J	301	-	4,4,4	0.54	0	6,6,6	0.25	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	SO4	A	301	-	-	0/0/0/0	0/0/0/0
6	SO4	A	302	-	-	0/0/0/0	0/0/0/0
6	SO4	A	303	-	-	0/0/0/0	0/0/0/0
6	SO4	D	301	-	-	0/0/0/0	0/0/0/0
6	SO4	F	301	-	-	0/0/0/0	0/0/0/0
6	SO4	F	302	-	-	0/0/0/0	0/0/0/0
6	SO4	I	301	-	-	0/0/0/0	0/0/0/0
6	SO4	J	301	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	302	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

### 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<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%)	0.24	10 (3%) 43 45	29, 55, 106, 134	0
1	F	276/276 (100%)	0.23	7 (2%) 58 59	30, 62, 104, 116	0
2	B	100/100 (100%)	-0.01	1 (1%) 82 83	31, 49, 77, 93	0
2	G	100/100 (100%)	0.04	2 (2%) 65 66	33, 51, 74, 101	0
3	C	10/10 (100%)	0.07	0 100 100	36, 37, 41, 50	0
3	H	10/10 (100%)	0.20	0 100 100	37, 41, 51, 55	0
4	D	197/200 (98%)	0.76	29 (14%) 3 2	33, 65, 134, 149	0
4	I	200/200 (100%)	0.67	20 (10%) 8 7	31, 68, 129, 144	0
5	E	244/246 (99%)	0.48	15 (6%) 22 22	27, 61, 123, 154	0
5	J	246/246 (100%)	0.08	3 (1%) 79 80	28, 52, 94, 121	0
All	All	1659/1664 (99%)	0.34	87 (5%) 28 29	27, 57, 120, 154	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	165	SER	9.9
4	D	148	SER	6.8
5	E	246	ASP	6.4
4	I	202	PRO	5.8
4	I	166	MET	5.4
4	I	127	LYS	5.2
4	I	164	ARG	5.2
4	I	128	SER	5.1
4	I	195	GLU	4.7
1	A	197	HIS	4.7
4	D	198	PHE	4.4
4	D	149	LYS	4.4
5	E	40	MET	4.3

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Mol	Chain	Res	Type	RSRZ
4	I	201	SER	4.2
4	I	165	SER	4.2
4	I	184	CYS	4.1
5	E	203	TRP	4.0
2	G	0	MET	4.0
1	A	248	VAL	4.0
4	D	192	ILE	3.6
1	A	195	SER	3.6
4	D	193	ILE	3.5
1	A	194	VAL	3.4
4	D	134	CYS	3.3
4	D	133	VAL	3.3
5	E	138	SER	3.3
4	I	162	ASP	3.2
4	D	135	LEU	3.2
4	D	147	GLN	3.2
2	B	99	MET	3.1
1	F	230	LEU	3.1
5	E	134	GLU	3.1
4	D	189	ASN	3.1
1	A	251	SER	3.1
4	D	181	ASP	3.1
5	E	210	PHE	3.0
5	E	135	ALA	3.0
2	G	99	MET	3.0
4	D	197	THR	3.0
4	D	168	PHE	2.9
4	D	121	TYR	2.9
1	A	196	ASP	2.9
5	E	148	LEU	2.9
4	D	176	TRP	2.9
4	D	166	MET	2.8
4	D	136	PHE	2.8
4	I	168	PHE	2.8
4	I	123	LEU	2.8
5	E	245	ALA	2.7
1	A	276	PRO	2.7
4	D	123	LEU	2.7
4	D	199	PHE	2.7
5	E	128	ALA	2.7
4	D	187	ALA	2.6
4	D	151	SER	2.6

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Mol	Chain	Res	Type	RSRZ
4	D	130	ASP	2.6
4	D	128	SER	2.5
5	E	144	THR	2.5
4	I	178	ASN	2.5
1	F	209	TYR	2.5
4	I	196	ASP	2.5
4	I	198	PHE	2.5
4	D	164	ARG	2.5
4	I	194	PRO	2.5
4	D	194	PRO	2.4
5	J	246	ASP	2.4
4	I	142	GLN	2.4
4	D	180	SER	2.3
1	A	252	GLY	2.3
1	A	256	ARG	2.3
5	J	207	ARG	2.3
4	I	53	SER	2.3
1	F	255	GLN	2.2
4	I	167	ASP	2.2
1	F	247	VAL	2.2
1	F	180	GLN	2.1
5	E	179	LEU	2.1
1	F	227	ASP	2.1
5	J	134	GLU	2.1
1	A	228	THR	2.1
5	E	185	LEU	2.1
5	E	165	GLY	2.1
4	D	162	ASP	2.1
4	D	122	GLN	2.1
1	F	217	TRP	2.1
4	I	188	PHE	2.0
5	E	237	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	D	301	5/5	0.82	0.33	10.76	109,115,122,129	0
6	SO4	A	303	5/5	0.87	0.35	8.54	93,103,115,116	0
6	SO4	F	301	5/5	0.94	0.40	8.02	67,72,87,92	0
6	SO4	I	301	5/5	0.85	0.32	4.66	117,130,137,138	0
6	SO4	A	301	5/5	0.87	0.19	1.12	76,77,82,85	0
6	SO4	F	302	5/5	0.89	0.15	0.24	74,76,79,84	0
6	SO4	J	301	5/5	0.89	0.16	-0.36	79,89,96,97	0
6	SO4	A	302	5/5	0.86	0.27	-	84,99,103,104	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.