



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:39 pm BST

PDB ID : 2ZOK
Title : Crystal structure of H-2Db in complex with JHMV epitope S510
Authors : Theodossis, A.; Dunstone, M.A.; Rossjohn, J.
Deposited on : 2008-05-22
Resolution : 2.10 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

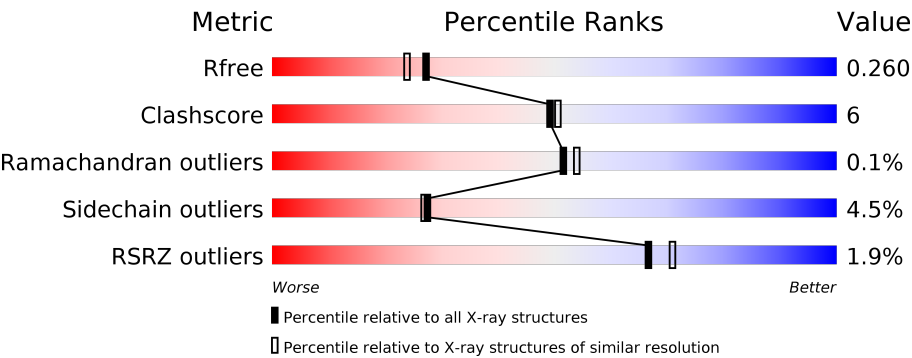
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	278	<div><div>3%</div><div></div><div>76%</div><div>12%</div><div>•</div><div>9%</div></div>
1	C	278	<div><div>%</div><div></div><div>78%</div><div>14%</div><div>•</div><div>7%</div></div>
1	E	278	<div><div>3%</div><div></div><div>74%</div><div>15%</div><div>•</div><div>9%</div></div>
1	G	278	<div><div>2%</div><div></div><div>83%</div><div>10%</div><div>•</div><div>5%</div></div>
2	B	100	<div><div></div><div></div><div>88%</div><div>10%</div><div>••</div></div>
2	D	100	<div><div>%</div><div></div><div>81%</div><div>16%</div><div>••</div></div>

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Mol	Chain	Length	Quality of chain
2	F	100	
2	H	100	
3	I	9	
3	J	9	
3	K	9	
3	L	9	

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
4	SO4	I	10[B]	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13084 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2088	1323	371	385	9			
1	C	258	Total	C	N	O	S	0	0	0
			2140	1356	378	397	9			
1	E	253	Total	C	N	O	S	0	0	0
			2096	1328	375	385	8			
1	G	263	Total	C	N	O	S	0	0	0
			2165	1372	382	402	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	276	ARG	-	expression tag	UNP P01899
A	277	TRP	-	expression tag	UNP P01899
A	278	GLU	-	expression tag	UNP P01899
C	276	ARG	-	expression tag	UNP P01899
C	277	TRP	-	expression tag	UNP P01899
C	278	GLU	-	expression tag	UNP P01899
E	276	ARG	-	expression tag	UNP P01899
E	277	TRP	-	expression tag	UNP P01899
E	278	GLU	-	expression tag	UNP P01899
G	276	ARG	-	expression tag	UNP P01899
G	277	TRP	-	expression tag	UNP P01899
G	278	GLU	-	expression tag	UNP P01899

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	D	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	H	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P01887
D	0	MET	-	initiating methionine	UNP P01887
F	0	MET	-	initiating methionine	UNP P01887
H	0	MET	-	initiating methionine	UNP P01887

- Molecule 3 is a protein called 9-meric peptide from Spike glycoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	9	Total	C	N	O	0	0	0
			72	47	13	12			
3	L	9	Total	C	N	O	0	0	0
			72	47	13	12			
3	J	9	Total	C	N	O	0	0	0
			72	47	13	12			
3	K	9	Total	C	N	O	0	0	0
			72	47	13	12			

There are 4 discrepancies between the modelled and reference sequences:

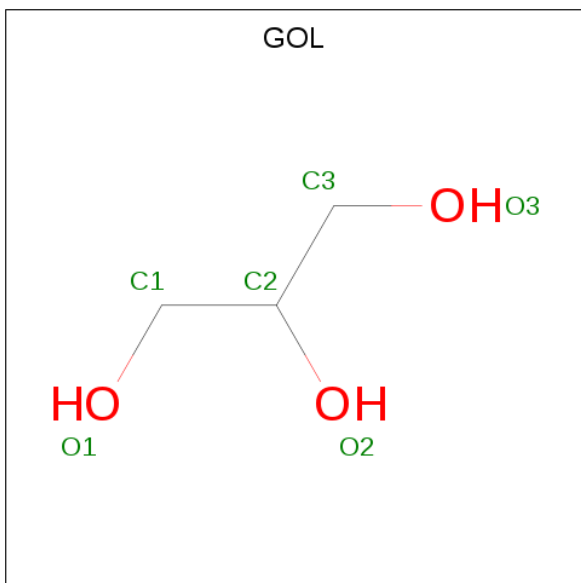
Chain	Residue	Modelled	Actual	Comment	Reference
I	1	ABA	CYS	modified residue	UNP Q02385
L	1	ABA	CYS	modified residue	UNP Q02385
J	1	ABA	CYS	modified residue	UNP Q02385
K	1	ABA	CYS	modified residue	UNP Q02385

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	1
			10	8	2		
4	I	1	Total	O	S	0	1
			10	8	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0

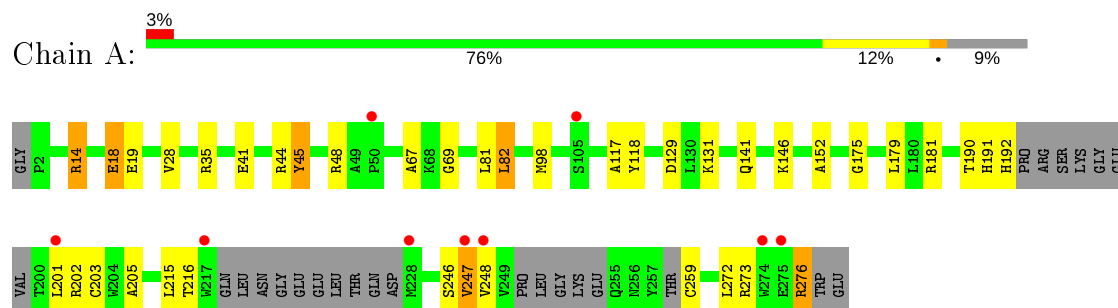
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	171	Total O 171 171	0	0
6	B	78	Total O 78 78	0	0
6	C	163	Total O 163 163	0	0
6	D	73	Total O 73 73	0	0
6	E	163	Total O 163 163	0	0
6	F	74	Total O 74 74	0	0
6	G	143	Total O 143 143	0	0
6	H	88	Total O 88 88	0	0
6	I	4	Total O 4 4	0	0
6	L	3	Total O 3 3	0	0
6	J	3	Total O 3 3	0	0
6	K	6	Total O 6 6	0	0

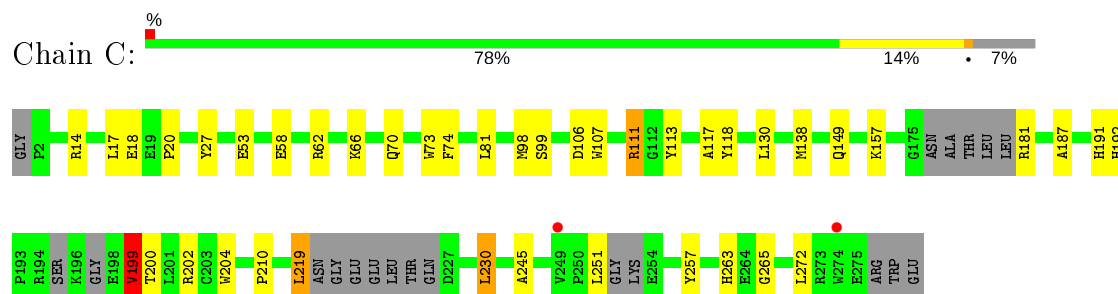
3 Residue-property plots [i](#)

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.

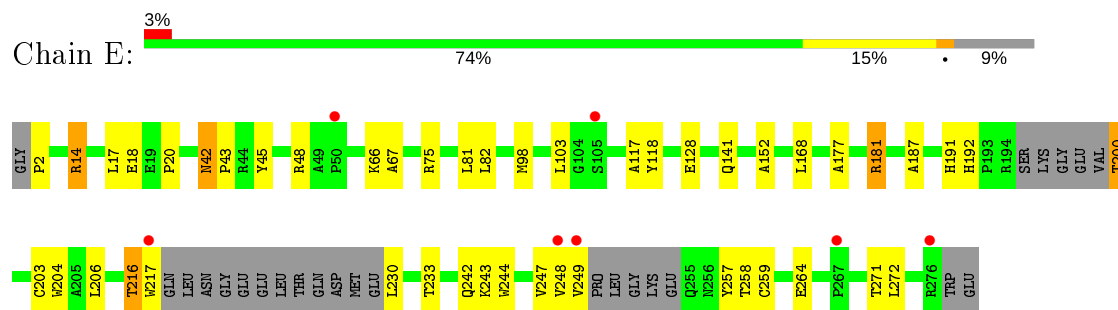
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



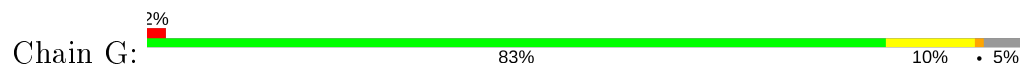
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain





- Molecule 2: Beta-2-microglobulin

Chain B: 88% 10% ..



- Molecule 2: Beta-2-microglobulin

Chain D: 81% 16% ..



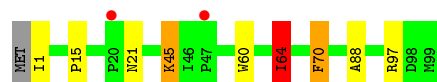
- Molecule 2: Beta-2-microglobulin

Chain F: 83% 12% ..



- Molecule 2: Beta-2-microglobulin

Chain H: 90% 6% ...



- Molecule 3: 9-meric peptide from Spike glycoprotein

Chain I: 78% 22%




- Molecule 3: 9-meric peptide from Spike glycoprotein

Chain L: 78% 22%




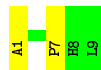
- Molecule 3: 9-meric peptide from Spike glycoprotein

Chain J:  78% 22%



- Molecule 3: 9-meric peptide from Spike glycoprotein

Chain K:  78% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.54Å 86.06Å 152.07Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	56.98 – 2.10 56.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (56.98-2.10) 95.0 (56.98-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.266 0.202 , 0.260	Depositor DCC
R_{free} test set	5737 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13084	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9892e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: ABA, 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	0.93	2/2148 (0.1%)	0.85	3/2910 (0.1%)
1	C	0.91	1/2201 (0.0%)	0.87	3/2981 (0.1%)
1	E	0.95	0/2158	0.86	2/2927 (0.1%)
1	G	0.93	0/2229	0.87	3/3024 (0.1%)
2	B	0.97	1/847 (0.1%)	0.84	0/1148
2	D	0.92	0/847	0.81	0/1148
2	F	0.93	0/847	0.83	0/1148
2	H	0.93	0/847	0.82	1/1148 (0.1%)
3	I	0.99	0/69	0.92	0/93
3	J	0.93	0/69	0.84	0/93
3	K	0.79	0/69	0.86	0/93
3	L	1.10	0/69	0.89	0/93
All	All	0.93	4/12400 (0.0%)	0.85	12/16806 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	27	VAL	CB-CG1	5.34	1.64	1.52
1	A	28	VAL	CB-CG1	5.19	1.63	1.52
1	C	73	TRP	CB-CG	5.17	1.59	1.50
1	A	45	TYR	CD2-CE2	5.11	1.47	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	G	251	LEU	CA-CB-CG	7.01	131.43	115.30
1	E	14	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	A	82	LEU	CA-CB-CG	6.71	130.72	115.30
1	A	35	ARG	NE-CZ-NH2	-6.20	117.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	VAL	CB-CA-C	-6.20	99.61	111.40
2	H	64	ILE	CG1-CB-CG2	-5.92	98.39	111.40
1	C	230	LEU	CA-CB-CG	5.84	128.73	115.30
1	C	62	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	E	82	LEU	CA-CB-CG	5.19	127.24	115.30
1	G	75	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	G	62	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2088	0	1962	29	0
1	C	2140	0	2008	24	0
1	E	2096	0	1973	28	0
1	G	2165	0	2040	22	0
2	B	821	0	796	8	0
2	D	821	0	796	13	0
2	F	821	0	796	10	0
2	H	821	0	796	7	0
3	I	72	0	68	3	0
3	J	72	0	68	2	0
3	K	72	0	68	2	0
3	L	72	0	68	2	0
4	A	5	0	0	0	0
4	E	5	0	0	0	0
4	G	10	0	0	1	0
4	I	10	0	0	4	0
5	A	6	0	8	0	0
5	C	6	0	8	1	0
5	E	6	0	8	0	0
5	G	6	0	8	1	0
6	A	171	0	0	6	0
6	B	78	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	163	0	0	3	0
6	D	73	0	0	0	0
6	E	163	0	0	3	0
6	F	74	0	0	1	0
6	G	143	0	0	3	0
6	H	88	0	0	1	0
6	I	4	0	0	0	0
6	J	3	0	0	0	0
6	K	6	0	0	0	0
6	L	3	0	0	0	0
All	All	13084	0	11471	134	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 6.

All (134) 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:A:203:CYS:HG	1:A:259:CYS:HG	1.10	0.97
1:A:201:LEU:O	1:A:246:SER:HA	1.81	0.80
1:G:199:VAL:HG22	1:G:251:LEU:HD13	1.65	0.79
1:C:199:VAL:HG22	1:C:251:LEU:HD13	1.66	0.78
2:B:37:ILE:HD11	2:B:64:ILE:HG21	1.68	0.75
1:A:175:GLY:O	1:A:179:LEU:HG	1.87	0.73
1:A:203:CYS:CB	1:A:259:CYS:HG	2.02	0.72
2:D:1:ILE:HG23	2:D:2:GLN:H	1.55	0.70
1:G:263:HIS:CD2	1:G:265:GLY:H	2.11	0.68
1:G:263:HIS:HD2	1:G:265:GLY:H	1.40	0.67
2:D:7:ILE:HD12	2:D:91:LYS:HD3	1.75	0.67
1:C:263:HIS:HD2	1:C:265:GLY:H	1.43	0.66
1:G:146:LYS:HE3	4:G:279[A]:SO4:O3	1.96	0.66
1:E:191:HIS:HD2	1:E:192:HIS:N	1.94	0.65
2:H:45:LYS:HB3	2:H:45:LYS:NZ	2.11	0.65
1:E:141:GLN:HE21	2:H:88:ALA:HB1	1.62	0.63
1:G:98:MET:CE	6:G:326:HOH:O	2.47	0.63
2:B:37:ILE:CD1	2:B:64:ILE:HG21	2.29	0.63
1:G:111:ARG:HD2	1:G:113:TYR:CZ	2.34	0.62
1:C:27:TYR:CG	5:C:279:GOL:H31	2.34	0.61
1:A:98:MET:HE3	6:A:394:HOH:O	1.99	0.61
1:A:146:LYS:HE2	4:I:10[B]:SO4:O2	2.02	0.60
1:C:210:PRO:O	1:C:263:HIS:HE1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:ILE:CD1	2:F:64:ILE:HG21	2.32	0.59
1:C:263:HIS:CD2	1:C:265:GLY:H	2.20	0.59
1:A:203:CYS:CB	1:A:259:CYS:SG	2.91	0.59
1:C:191:HIS:CE1	1:C:199:VAL:HG11	2.38	0.59
1:G:210:PRO:O	1:G:263:HIS:HE1	1.85	0.59
2:D:37:ILE:CD1	2:D:64:ILE:HG21	2.33	0.58
1:G:98:MET:HE1	6:G:326:HOH:O	2.02	0.58
1:E:249:VAL:HG11	1:E:257:TYR:CZ	2.39	0.58
1:A:146:LYS:CE	4:I:10[B]:SO4:O2	2.51	0.57
1:G:146:LYS:HE2	3:L:8:HIS:O	2.04	0.57
1:A:41:GLU:H	1:A:41:GLU:CD	2.08	0.57
1:C:98:MET:HE1	6:C:292:HOH:O	2.04	0.57
1:E:249:VAL:CG1	1:E:257:TYR:CZ	2.88	0.56
1:A:98:MET:HE1	6:A:302:HOH:O	2.04	0.56
1:A:131:LYS:NZ	6:A:384:HOH:O	2.34	0.56
2:D:1:ILE:HG23	2:D:2:GLN:N	2.20	0.56
1:E:42:ASN:HD22	1:E:42:ASN:C	2.08	0.56
1:A:98:MET:CE	6:A:394:HOH:O	2.53	0.55
1:E:14:ARG:HD3	1:E:18:GLU:HB3	1.88	0.55
1:E:42:ASN:C	1:E:42:ASN:ND2	2.60	0.55
2:D:21:ASN:O	2:D:22:ILE:HG13	2.06	0.55
1:G:187:ALA:CB	1:G:272:LEU:HD21	2.36	0.55
2:D:37:ILE:HD12	2:D:64:ILE:HG21	1.89	0.55
1:E:98:MET:CE	6:E:318:HOH:O	2.56	0.54
3:I:7:PRO:HB3	4:I:10[B]:SO4:O2	2.07	0.54
1:E:191:HIS:CD2	1:E:192:HIS:N	2.75	0.54
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.42	0.54
1:E:177:ALA:O	1:E:181:ARG:HG2	2.08	0.53
1:G:27:TYR:CG	5:G:280:GOL:H31	2.43	0.53
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.44	0.52
2:F:1:ILE:HD12	6:F:123:HOH:O	2.08	0.52
2:F:37:ILE:CD1	2:F:64:ILE:CG2	2.87	0.52
1:C:98:MET:CE	6:C:292:HOH:O	2.58	0.52
1:G:133:TRP:HB2	1:G:144:ARG:HG3	1.92	0.52
2:B:37:ILE:HD11	2:B:64:ILE:CG2	2.37	0.52
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.45	0.51
1:E:244:TRP:HZ2	2:F:99:MET:HE3	1.75	0.51
1:A:129:ASP:O	1:A:131:LYS:HG3	2.10	0.51
2:H:1:ILE:HG12	6:H:176:HOH:O	2.10	0.51
1:A:18:GLU:HB2	6:A:433:HOH:O	2.11	0.51
1:E:233:THR:OG1	1:E:243:LYS:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ALA:HB2	3:I:7:PRO:HG2	1.93	0.50
1:E:98:MET:HE1	6:E:306:HOH:O	2.11	0.49
1:A:191:HIS:CD2	1:A:192:HIS:N	2.81	0.49
1:C:106:ASP:O	1:C:107:TRP:HB2	2.11	0.49
2:D:37:ILE:CD1	2:D:64:ILE:CG2	2.91	0.49
1:E:81:LEU:HD13	1:E:118:TYR:CD1	2.48	0.49
2:D:21:ASN:HB3	2:D:70:PHE:CE1	2.48	0.48
1:A:98:MET:CE	6:A:302:HOH:O	2.62	0.48
1:C:111:ARG:HG3	1:C:113:TYR:CE1	2.48	0.48
1:A:205:ALA:HB2	1:A:215:LEU:HD21	1.96	0.48
1:G:187:ALA:HB3	1:G:272:LEU:HD21	1.95	0.48
1:E:103:LEU:HG	1:E:168:LEU:HD23	1.96	0.48
1:C:187:ALA:HA	1:C:204:TRP:O	2.14	0.47
1:G:199:VAL:CG2	1:G:251:LEU:HD13	2.38	0.47
1:A:14:ARG:HD2	1:A:19:GLU:O	2.15	0.47
1:A:45:TYR:CE2	1:A:67:ALA:HB2	2.50	0.47
1:C:18:GLU:O	1:C:20:PRO:HD3	2.14	0.46
1:E:48:ARG:NH2	2:F:53:ASP:OD2	2.47	0.46
1:E:206:LEU:HD23	1:E:242:GLN:HB3	1.97	0.46
2:B:37:ILE:CD1	2:B:64:ILE:CG2	2.92	0.46
1:E:42:ASN:HD22	1:E:43:PRO:N	2.13	0.46
1:G:98:MET:HE2	6:G:326:HOH:O	2.11	0.46
3:J:3:LEU:H	3:J:3:LEU:HD23	1.81	0.46
1:A:276:ARG:HD2	1:A:276:ARG:HA	1.76	0.46
1:A:216:THR:O	1:A:259:CYS:HA	2.17	0.45
1:A:48:ARG:NH2	2:B:53:ASP:OD2	2.47	0.45
1:C:202:ARG:HG2	1:C:204:TRP:NE1	2.32	0.45
1:G:81:LEU:HD13	1:G:118:TYR:CD1	2.51	0.45
1:E:20:PRO:HD2	1:E:75:ARG:HG2	1.99	0.45
1:G:250:PRO:HB2	1:G:253:LYS:HB2	1.99	0.45
1:A:146:LYS:HE3	4:I:10[B]:SO4:O2	2.16	0.45
1:E:187:ALA:HA	1:E:204:TRP:O	2.17	0.45
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.52	0.44
1:C:130:LEU:HB2	1:C:157:LYS:HD2	1.99	0.44
1:C:187:ALA:CB	1:C:272:LEU:HD21	2.47	0.44
1:E:98:MET:HE3	6:E:318:HOH:O	2.14	0.44
2:D:15:PRO:HG3	2:D:97:ARG:HG3	2.00	0.44
1:C:70:GLN:O	1:C:74:PHE:HD1	2.02	0.43
1:C:230:LEU:HD12	1:C:245:ALA:HB2	2.00	0.43
1:E:66:LYS:NZ	3:K:1:ABA:HG3	2.33	0.43
2:F:17:ASN:OD1	2:F:97:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:ALA:HB2	3:K:7:PRO:HG2	2.01	0.43
1:E:200:THR:HA	1:E:247:VAL:O	2.18	0.43
1:A:69:GLY:HA3	3:I:4:TRP:CZ3	2.54	0.43
1:A:247:VAL:HB	1:A:248:VAL:H	1.69	0.43
1:G:187:ALA:HA	1:G:204:TRP:O	2.19	0.43
2:B:85:ASP:OD1	1:C:138:MET:SD	2.77	0.42
2:F:40:LEU:HD23	2:F:45:LYS:HA	2.02	0.42
1:C:58:GLU:HB2	6:C:359:HOH:O	2.18	0.42
1:C:66:LYS:NZ	3:J:1:ABA:HG3	2.34	0.42
2:D:40:LEU:HD23	2:D:45:LYS:HA	2.00	0.42
2:H:15:PRO:CG	2:H:97:ARG:HG3	2.50	0.42
2:H:64:ILE:HG21	2:H:64:ILE:HD13	1.59	0.42
1:E:45:TYR:CE2	1:E:67:ALA:HB2	2.55	0.42
1:G:206:LEU:HD23	1:G:242:GLN:HB3	2.02	0.42
1:E:216:THR:O	1:E:259:CYS:HA	2.20	0.41
2:F:69:GLU:HG2	2:F:69:GLU:H	1.55	0.41
1:E:117:ALA:HB2	2:F:60:TRP:CE2	2.55	0.41
1:E:203:CYS:HB2	1:E:217:TRP:CZ2	2.55	0.41
1:C:192:HIS:HB2	1:C:200:THR:HB	2.03	0.41
1:C:219:LEU:HG	1:C:257:TYR:CE2	2.55	0.41
2:B:32:PRO:HB2	2:B:33:PRO:HD2	2.03	0.41
1:C:81:LEU:HD13	1:C:118:TYR:CD1	2.56	0.41
2:D:1:ILE:CG2	2:D:2:GLN:H	2.30	0.41
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.21	0.41
1:G:147:TRP:CZ2	3:L:9:LEU:HD23	2.55	0.41
2:F:6:GLN:HG2	2:F:29:GLN:HG3	2.03	0.40
1:G:144:ARG:NE	1:G:148:GLU:OE2	2.45	0.40
2:H:21:ASN:HB3	2:H:70:PHE:CE1	2.55	0.40
2:D:11:SER:HA	2:D:22:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	242/278 (87%)	238 (98%)	4 (2%)	0	100	100
1	C	247/278 (89%)	244 (99%)	3 (1%)	0	100	100
1	E	245/278 (88%)	242 (99%)	3 (1%)	0	100	100
1	G	257/278 (92%)	252 (98%)	4 (2%)	1 (0%)	34	32
2	B	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
2	D	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
2	F	97/100 (97%)	91 (94%)	6 (6%)	0	100	100
2	H	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	J	7/9 (78%)	7 (100%)	0	0	100	100
3	K	7/9 (78%)	7 (100%)	0	0	100	100
3	L	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1407/1548 (91%)	1377 (98%)	29 (2%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	176	ASN

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	214/236 (91%)	205 (96%)	9 (4%)	30	30
1	C	221/236 (94%)	212 (96%)	9 (4%)	30	31
1	E	215/236 (91%)	202 (94%)	13 (6%)	19	16
1	G	223/236 (94%)	215 (96%)	8 (4%)	35	36
2	B	94/95 (99%)	90 (96%)	4 (4%)	29	29
2	D	94/95 (99%)	89 (95%)	5 (5%)	22	20
2	F	94/95 (99%)	87 (93%)	7 (7%)	13	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	94/95 (99%)	91 (97%)	3 (3%)	39	41
3	I	7/7 (100%)	7 (100%)	0	100	100
3	J	7/7 (100%)	7 (100%)	0	100	100
3	K	7/7 (100%)	7 (100%)	0	100	100
3	L	7/7 (100%)	7 (100%)	0	100	100
All	All	1277/1352 (94%)	1219 (96%)	58 (4%)	27	27

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	44	ARG
1	A	82	LEU
1	A	141	GLN
1	A	181	ARG
1	A	247	VAL
1	A	272	LEU
1	A	273	ARG
1	A	276	ARG
2	B	22	ILE
2	B	45	LYS
2	B	64	ILE
2	B	70	PHE
1	C	14	ARG
1	C	17	LEU
1	C	53	GLU
1	C	99	SER
1	C	111	ARG
1	C	149	GLN
1	C	181	ARG
1	C	199	VAL
1	C	219	LEU
2	D	16	GLU
2	D	64	ILE
2	D	69	GLU
2	D	70	PHE
2	D	89	GLU
1	E	2	PRO
1	E	17	LEU
1	E	42	ASN

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Mol	Chain	Res	Type
1	E	128	GLU
1	E	181	ARG
1	E	200	THR
1	E	216	THR
1	E	230	LEU
1	E	248	VAL
1	E	258	THR
1	E	264	GLU
1	E	271	THR
1	E	272	LEU
2	F	1	ILE
2	F	22	ILE
2	F	29	GLN
2	F	51	MET
2	F	64	ILE
2	F	70	PHE
2	F	97	ARG
1	G	17	LEU
1	G	41	GLU
1	G	111	ARG
1	G	145	ARG
1	G	176	ASN
1	G	199	VAL
1	G	218	GLN
1	G	251	LEU
2	H	45	LYS
2	H	64	ILE
2	H	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	115	GLN
1	A	141	GLN
1	A	191	HIS
1	A	255	GLN
1	C	115	GLN
1	C	191	HIS
1	C	263	HIS
2	D	38	GLN
1	E	42	ASN

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Mol	Chain	Res	Type
1	E	54	GLN
1	E	72	GLN
1	E	115	GLN
1	E	141	GLN
1	E	191	HIS
1	G	115	GLN
1	G	149	GLN
1	G	263	HIS
2	H	17	ASN
2	H	29	GLN
2	H	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	ABA	L	1	3	4,5,6	0.51	0	1,5,7	0.27	0
3	ABA	J	1	3	4,5,6	0.60	0	1,5,7	0.25	0
3	ABA	K	1	3	4,5,6	0.50	0	1,5,7	0.51	0
3	ABA	I	1	3	4,5,6	0.74	0	1,5,7	0.19	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
3	ABA	L	1	3	-	0/3/4/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ABA	J	1	3	-	1/3/4/6	-
3	ABA	K	1	3	-	2/3/4/6	-
3	ABA	I	1	3	-	0/3/4/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1	ABA	C-CA-CB-CG
3	K	1	ABA	N-CA-CB-CG
3	J	1	ABA	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1	ABA	1	0
3	K	1	ABA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
4	SO4	A	279	-	4,4,4	0.46	0	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	E	279	-	4,4,4	0.57	0	6,6,6	1.17	0
4	SO4	G	279[A]	-	4,4,4	0.41	0	6,6,6	1.17	1 (16%)
5	GOL	G	280	-	5,5,5	0.49	0	5,5,5	1.32	0
5	GOL	E	280	-	5,5,5	0.37	0	5,5,5	0.54	0
5	GOL	C	279	-	5,5,5	0.40	0	5,5,5	0.73	0
5	GOL	A	280	-	5,5,5	0.23	0	5,5,5	0.93	0
4	SO4	I	10[A]	-	4,4,4	0.41	0	6,6,6	1.14	1 (16%)
4	SO4	I	10[B]	-	4,4,4	0.10	0	6,6,6	1.07	0
4	SO4	G	279[B]	-	4,4,4	0.19	0	6,6,6	1.43	1 (16%)

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
5	GOL	E	280	-	-	2/4/4/4	-
5	GOL	C	279	-	-	4/4/4/4	-
5	GOL	A	280	-	-	3/4/4/4	-
5	GOL	G	280	-	-	4/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	279[B]	SO4	O4-S-O3	2.59	120.10	109.06
4	G	279[A]	SO4	O4-S-O3	-2.49	98.43	109.06
4	I	10[A]	SO4	O4-S-O3	-2.36	98.97	109.06

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	279	GOL	O1-C1-C2-C3
5	G	280	GOL	O1-C1-C2-C3
5	E	280	GOL	C1-C2-C3-O3
5	G	280	GOL	O2-C2-C3-O3
5	C	279	GOL	O1-C1-C2-O2
5	G	280	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	E	280	GOL	O2-C2-C3-O3
5	C	279	GOL	O2-C2-C3-O3
5	A	280	GOL	O1-C1-C2-O2
5	A	280	GOL	O2-C2-C3-O3
5	G	280	GOL	C1-C2-C3-O3
5	C	279	GOL	C1-C2-C3-O3
5	A	280	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	279[A]	SO4	1	0
5	G	280	GOL	1	0
5	C	279	GOL	1	0
4	I	10[B]	SO4	4	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, 95th 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	252/278 (90%)	-0.07	9 (3%) 42 49	9, 26, 56, 70	15 (5%)
1	C	258/278 (92%)	-0.14	2 (0%) 86 88	10, 25, 49, 59	10 (3%)
1	E	253/278 (91%)	-0.01	7 (2%) 53 59	8, 24, 58, 74	13 (5%)
1	G	263/278 (94%)	-0.08	5 (1%) 66 71	9, 25, 51, 60	17 (6%)
2	B	99/100 (99%)	-0.19	0 100 100	13, 26, 40, 45	6 (6%)
2	D	99/100 (99%)	0.03	1 (1%) 82 85	13, 28, 44, 47	6 (6%)
2	F	99/100 (99%)	-0.04	1 (1%) 82 85	13, 26, 41, 45	7 (7%)
2	H	99/100 (99%)	-0.05	2 (2%) 65 69	14, 27, 43, 53	6 (6%)
3	I	8/9 (88%)	-0.34	0 100 100	11, 13, 18, 21	0
3	J	8/9 (88%)	-0.42	0 100 100	12, 15, 21, 21	0
3	K	8/9 (88%)	-0.44	0 100 100	10, 13, 20, 20	0
3	L	8/9 (88%)	-0.42	0 100 100	12, 15, 20, 21	0
All	All	1454/1548 (93%)	-0.08	27 (1%) 66 71	8, 25, 50, 74	80 (5%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	248	VAL	4.2
1	E	276	ARG	4.1
1	G	250	PRO	3.8
1	G	249	VAL	3.8
1	G	274	TRP	3.8
1	C	249	VAL	3.8
1	A	247	VAL	3.7
1	A	217	TRP	3.4
1	A	275	GLU	3.1
1	G	199	VAL	2.7
1	E	249	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	248	VAL	2.6
2	F	1	ILE	2.5
2	H	20	PRO	2.5
1	C	274	TRP	2.5
1	A	201	LEU	2.5
1	A	105	SER	2.4
1	A	228	MET	2.4
1	E	217	TRP	2.3
1	A	274	TRP	2.3
2	H	47	PRO	2.3
2	D	1	ILE	2.2
1	A	50	PRO	2.2
1	A	248	VAL	2.1
1	E	267	PRO	2.1
1	E	50	PRO	2.1
1	E	105	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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
3	ABA	L	1	6/7	0.95	0.12	19,20,22,23	0
3	ABA	K	1	6/7	0.97	0.12	15,20,20,21	0
3	ABA	I	1	6/7	0.97	0.12	14,17,19,19	0
3	ABA	J	1	6/7	0.98	0.09	20,22,24,24	0

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. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
5	GOL	G	280	6/6	0.89	0.15	34,37,39,41	0
5	GOL	C	279	6/6	0.90	0.21	35,40,42,44	0
5	GOL	E	280	6/6	0.94	0.15	32,38,41,42	0
5	GOL	A	280	6/6	0.94	0.10	28,32,35,36	0
4	SO4	G	279[A]	5/5	0.95	0.19	5,9,18,24	5
4	SO4	G	279[B]	5/5	0.95	0.19	5,10,20,22	5
4	SO4	I	10[A]	5/5	0.97	0.20	6,11,19,22	5
4	SO4	I	10[B]	5/5	0.97	0.20	5,9,19,22	5
4	SO4	A	279	5/5	0.97	0.17	17,17,20,21	5
4	SO4	E	279	5/5	0.98	0.15	14,15,16,18	5

6.5 Other polymers [i](#)

There are no such residues in this entry.