



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:59 am GMT

PDB ID : 5E8N  
Title : The structure of the TEIPP associated Trh4 peptide in complex with H-2D(b)  
Authors : Hafstrand, I.; Doorduijn, E.; Duru, A.D.; Buratto, J.; Oliveira, C.C.; Sandalova, T.; van Hall, T.; Achour, A.  
Deposited on : 2015-10-14  
Resolution : 2.25 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

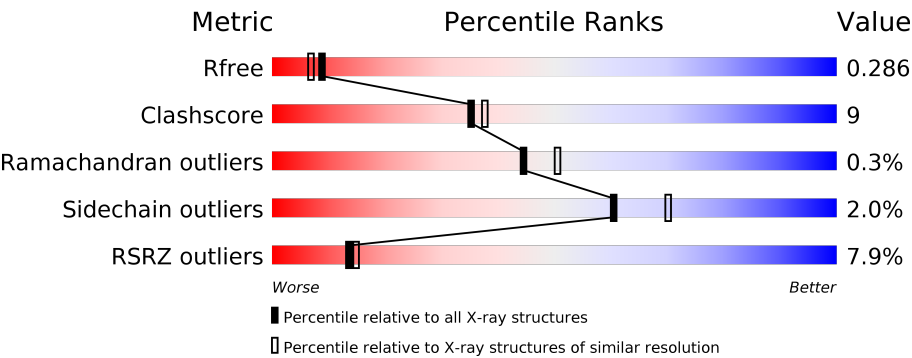
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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>9%</div><div><div></div><div>76%</div><div>22%</div><div>••</div></div></div>
1	D	276	<div><div>9%</div><div><div></div><div>77%</div><div>21%</div><div>•</div></div></div>
1	G	276	<div><div>7%</div><div><div></div><div>79%</div><div>18%</div><div>•</div></div></div>
1	J	276	<div><div>14%</div><div><div></div><div>68%</div><div>23%</div><div>• 7%</div></div></div>
2	B	99	<div><div>%</div><div><div></div><div>88%</div><div>12%</div><div></div></div></div>
2	E	99	<div><div>%</div><div><div></div><div>86%</div><div>14%</div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
2	H	99	<div><div>%</div><div><div></div><div>85%</div><div>15%</div></div></div>
2	K	99	<div><div>7%</div><div><div></div><div>74%</div><div>23%</div><div></div></div></div>
3	C	9	<div><div><div></div><div>67%</div><div>33%</div></div></div>
3	F	9	<div><div><div></div><div>78%</div><div>22%</div></div></div>
3	I	9	<div><div><div></div><div>67%</div><div>33%</div></div></div>
3	L	9	<div><div><div></div><div>22%</div><div>78%</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12495 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	272	Total	C	N	O	S	0	0	0
			2227	1408	391	419	9			
1	D	272	Total	C	N	O	S	0	1	0
			2237	1410	397	421	9			
1	G	269	Total	C	N	O	S	0	1	0
			2208	1394	389	416	9			
1	J	258	Total	C	N	O	S	0	0	0
			2113	1338	368	399	8			

- 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	1	0
			825	526	138	153	8			
2	E	99	Total	C	N	O	S	0	1	0
			821	523	137	153	8			
2	H	99	Total	C	N	O	S	0	1	0
			825	526	138	153	8			
2	K	99	Total	C	N	O	S	0	1	0
			817	520	136	153	8			

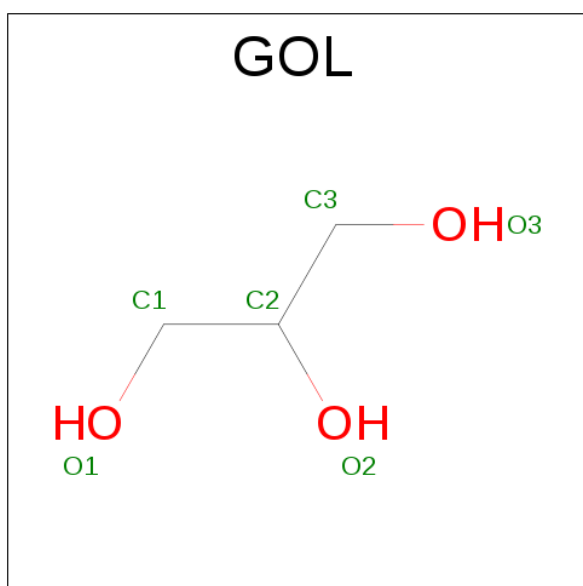
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ASP	ALA	conflict	UNP P01887
E	85	ASP	ALA	conflict	UNP P01887
H	85	ASP	ALA	conflict	UNP P01887
K	85	ASP	ALA	conflict	UNP P01887

- Molecule 3 is a protein called Ceramide synthase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			69	42	12	11	4			
3	F	9	Total	C	N	O	S	0	0	0
			69	42	12	11	4			
3	I	9	Total	C	N	O	S	0	0	0
			69	42	12	11	4			
3	L	9	Total	C	N	O	S	0	0	0
			69	42	12	11	4			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

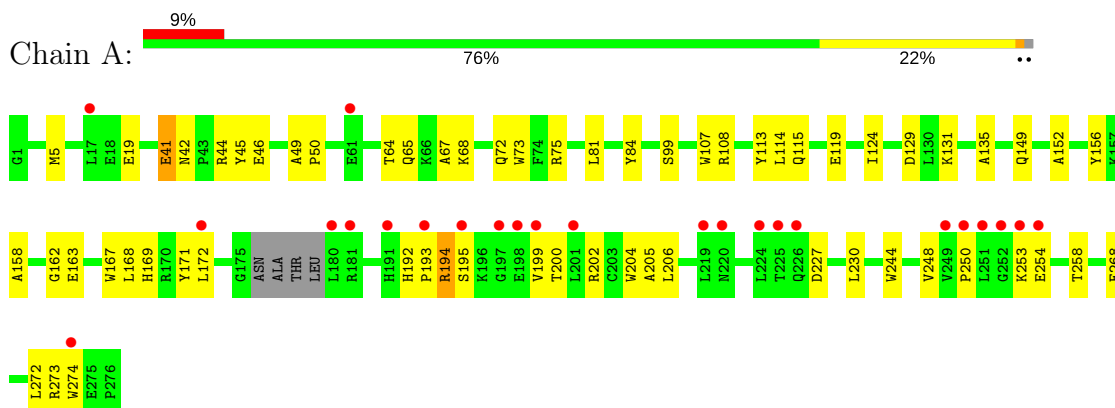
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		
6	B	22	Total	O	0	0
			22	22		
6	C	5	Total	O	0	0
			5	5		
6	D	22	Total	O	0	0
			22	22		
6	E	13	Total	O	0	0
			13	13		
6	F	5	Total	O	0	0
			5	5		
6	G	10	Total	O	0	0
			10	10		
6	H	17	Total	O	0	0
			17	17		
6	J	20	Total	O	0	0
			20	20		
6	K	1	Total	O	0	0
			1	1		
6	L	2	Total	O	0	0
			2	2		

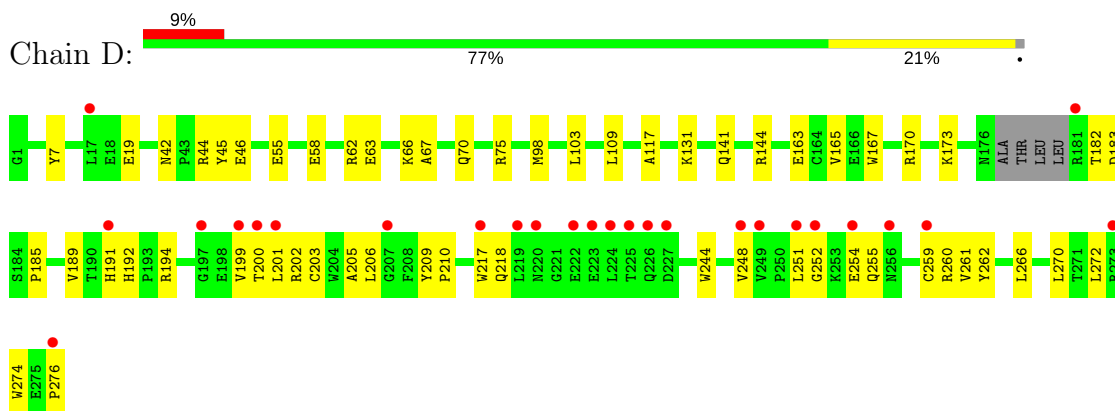
### 3 Residue-property plots [i](#)

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.

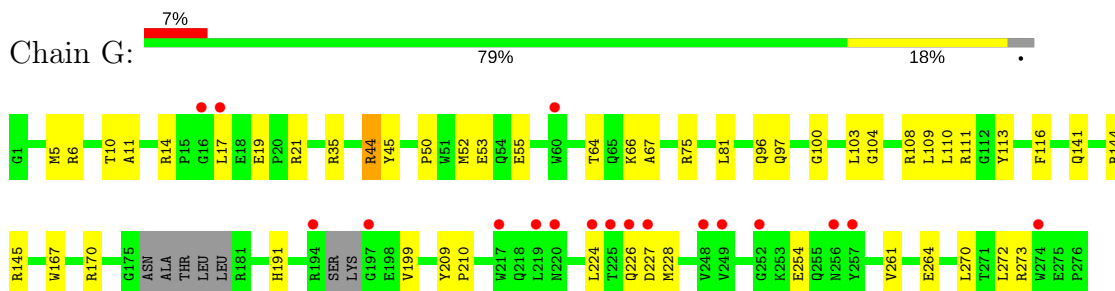
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



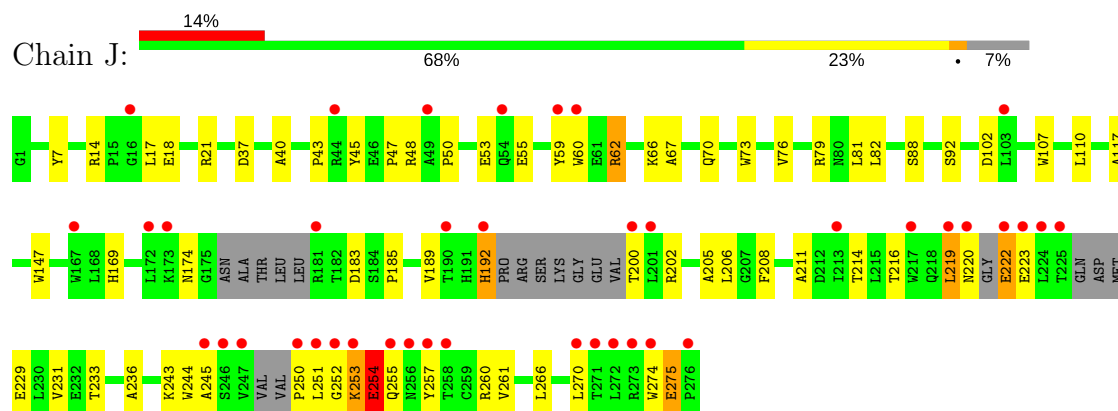
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



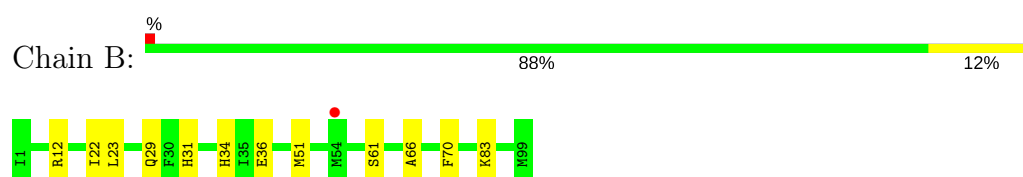
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



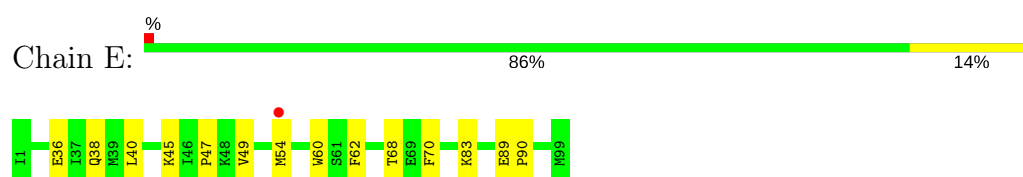
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



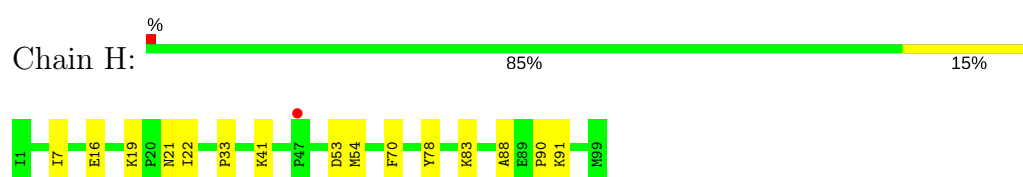
- Molecule 2: Beta-2-microglobulin



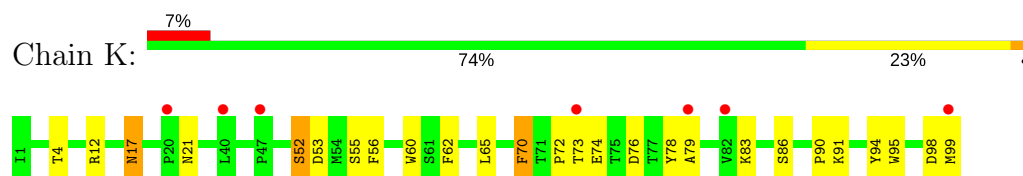
- Molecule 2: Beta-2-microglobulin



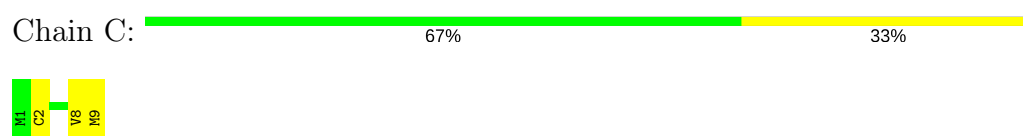
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin




- Molecule 3: Ceramide synthase 5



- Molecule 3: Ceramide synthase 5



Chain F:  78% 22%




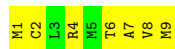
- Molecule 3: Ceramide synthase 5

Chain I:  67% 33%



- Molecule 3: Ceramide synthase 5

Chain L:  22% 78%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.51Å 124.25Å 99.29Å 90.00° 103.26° 90.00°	Depositor
Resolution (Å)	52.26 – 2.25 52.26 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.8 (52.26-2.25) 98.9 (52.26-2.25)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.25Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.239 , 0.286 0.238 , 0.286	Depositor DCC
$R_{free}$ test set	5032 reflections (4.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12495	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.73% 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	0.48	0/2293	0.65	1/3112 (0.0%)
1	D	0.49	0/2306	0.62	0/3129
1	G	0.42	0/2276	0.60	1/3089 (0.0%)
1	J	0.50	2/2173 (0.1%)	0.65	3/2945 (0.1%)
2	B	0.53	0/851	0.65	0/1154
2	E	0.48	0/847	0.66	0/1150
2	H	0.46	0/851	0.63	0/1154
2	K	0.44	0/843	0.66	0/1146
3	C	0.68	0/68	0.81	0/87
3	F	0.57	0/68	0.78	0/87
3	I	0.50	0/68	0.69	0/87
3	L	0.56	0/68	0.88	0/87
All	All	0.47	2/12712 (0.0%)	0.64	5/17227 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	275	GLU	CD-OE1	-6.01	1.19	1.25
1	J	18	GLU	C-N	5.41	1.46	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	LEU	CA-CB-CG	7.99	133.67	115.30
1	J	62	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	J	62	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	G	145	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	J	82	LEU	CA-CB-CG	5.03	126.86	115.30

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	2227	0	2089	44	0
1	D	2237	0	2089	49	0
1	G	2208	0	2053	34	0
1	J	2113	0	1956	62	1
2	B	825	0	793	8	0
2	E	821	0	782	12	0
2	H	825	0	793	8	1
2	K	817	0	771	18	0
3	C	69	0	79	3	0
3	F	69	0	79	3	0
3	I	69	0	79	3	0
3	L	69	0	79	9	0
4	B	6	0	8	2	0
5	G	5	0	0	0	0
6	A	18	0	0	2	0
6	B	22	0	0	1	0
6	C	5	0	0	0	0
6	D	22	0	0	0	0
6	E	13	0	0	0	0
6	F	5	0	0	0	0
6	G	10	0	0	0	0
6	H	17	0	0	0	0
6	J	20	0	0	2	0
6	K	1	0	0	0	0
6	L	2	0	0	0	0
All	All	12495	0	11650	224	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (224) 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:J:253:LYS:HD3	1:J:257:TYR:CE2	1.03	1.56
1:J:253:LYS:CD	1:J:257:TYR:CE2	1.87	1.52
1:J:253:LYS:CD	1:J:257:TYR:HE2	1.39	1.06
1:J:253:LYS:HD3	1:J:257:TYR:CD2	1.92	1.04
1:J:253:LYS:CD	1:J:257:TYR:CD2	2.40	1.04
1:J:220:ASN:HB3	1:J:222:GLU:N	1.73	1.03
1:D:251:LEU:HD12	1:D:254:GLU:OE2	1.62	1.00
1:J:250:PRO:N	1:J:253:LYS:HG2	1.78	0.97
1:J:253:LYS:CE	1:J:257:TYR:CE2	2.49	0.96
1:J:274:TRP:HD1	1:J:274:TRP:O	1.51	0.92
1:J:274:TRP:CD1	1:J:274:TRP:O	2.33	0.82
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.66	0.77
2:E:45:LYS:H	2:E:45:LYS:HD3	1.48	0.77
1:J:185:PRO:HB3	1:J:208:PHE:HB3	1.64	0.77
1:J:253:LYS:HD2	1:J:257:TYR:CD2	2.19	0.74
1:A:124:ILE:HG13	1:A:135:ALA:HB2	1.69	0.73
2:K:73:THR:OG1	2:K:76:ASP:OD2	2.08	0.72
2:H:83:LYS:HG2	2:H:90:PRO:HB3	1.72	0.72
1:J:274:TRP:CD1	1:J:274:TRP:C	2.63	0.71
1:G:55:GLU:OE1	1:G:170:ARG:NH2	2.25	0.69
1:D:251:LEU:CD1	1:D:254:GLU:OE2	2.38	0.69
1:J:70:GLN:OE1	3:L:4:ARG:NH1	2.28	0.66
1:J:88:SER:O	6:J:301:HOH:O	2.13	0.66
1:J:219:LEU:C	1:J:219:LEU:HD12	2.15	0.66
1:J:14:ARG:HB2	1:J:17:LEU:HD13	1.77	0.66
1:J:244:TRP:NE1	2:K:99:MET:O	2.29	0.66
1:A:119:GLU:OE1	6:A:301:HOH:O	2.13	0.66
1:A:73:TRP:CD1	3:C:8:VAL:HG12	2.31	0.65
1:J:253:LYS:HE3	1:J:257:TYR:CZ	2.33	0.64
1:J:253:LYS:HE3	1:J:257:TYR:CE2	2.30	0.64
1:J:66:LYS:NZ	3:L:1:MET:SD	2.71	0.64
1:G:141:GLN:OE1	1:G:144[B]:ARG:NH2	2.30	0.63
1:J:50:PRO:O	1:J:53:GLU:HG3	1.98	0.63
1:G:45:TYR:CE2	1:G:67:ALA:HB2	2.34	0.63
1:D:203:CYS:HB2	1:D:217:TRP:CZ2	2.34	0.62
2:H:7:ILE:HD12	2:H:91:LYS:HE3	1.82	0.62
1:A:119:GLU:HA	1:A:119:GLU:OE1	2.01	0.61
1:A:194:ARG:HG3	1:A:195:SER:H	1.66	0.60
1:J:250:PRO:N	1:J:253:LYS:HZ2	1.99	0.60
2:K:17:ASN:OD1	2:K:73:THR:HA	2.02	0.59
1:G:191:HIS:NE2	1:G:254:GLU:OE2	2.36	0.59
1:D:55:GLU:OE1	1:D:170:ARG:NH2	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:250:PRO:O	1:J:252:GLY:N	2.37	0.58
1:J:252:GLY:N	1:J:254:GLU:OE2	2.36	0.58
1:D:58:GLU:OE2	1:D:62:ARG:NH2	2.32	0.58
1:A:107:TRP:HE3	1:A:169:HIS:CD2	2.22	0.57
1:D:103:LEU:HD21	1:D:165:VAL:HG12	1.85	0.57
1:J:202:ARG:HD2	1:J:244:TRP:CD2	2.40	0.57
1:D:261:VAL:HB	1:D:270:LEU:HB2	1.86	0.57
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.39	0.57
1:D:218:GLN:HB2	1:D:260:ARG:HH21	1.69	0.57
2:K:17:ASN:O	2:K:72:PRO:O	2.23	0.57
2:K:17:ASN:ND2	2:K:74:GLU:HG3	2.20	0.57
1:D:191:HIS:NE2	1:D:199:VAL:HG21	2.21	0.56
2:E:45:LYS:H	2:E:45:LYS:CD	2.18	0.56
1:G:111:ARG:HD3	1:G:113:TYR:CZ	2.41	0.56
2:E:83:LYS:HG2	2:E:90:PRO:HB3	1.88	0.56
1:A:194:ARG:HD3	1:A:200:THR:HG23	1.88	0.56
1:G:50:PRO:O	1:G:53:GLU:HG3	2.06	0.55
1:A:200:THR:HG22	1:A:248:VAL:HG22	1.88	0.55
2:H:16:GLU:OE1	2:H:19:LYS:NZ	2.35	0.55
1:G:10:THR:HG23	1:G:96:GLN:HG2	1.89	0.55
1:A:194:ARG:HG3	1:A:195:SER:N	2.22	0.55
2:K:70:PHE:HD2	2:K:78:TYR:CZ	2.24	0.54
2:K:83:LYS:HG3	2:K:90:PRO:HG3	1.89	0.54
1:D:252:GLY:CA	1:D:254:GLU:OE1	2.56	0.54
1:A:108:ARG:HD3	1:D:262:TYR:CG	2.43	0.54
1:D:259:CYS:HB3	1:D:272:LEU:CD1	2.38	0.54
1:A:107:TRP:CE3	1:A:169:HIS:CD2	2.95	0.54
1:J:255:GLN:HG2	1:J:255:GLN:O	2.06	0.54
1:J:47:PRO:HG3	1:J:60:TRP:CZ2	2.43	0.53
2:K:78:TYR:O	2:K:95:TRP:N	2.37	0.53
1:A:107:TRP:HB3	1:A:169:HIS:NE2	2.22	0.53
1:A:193:PRO:HA	1:A:199:VAL:HG12	1.90	0.53
1:A:64:THR:HG22	1:A:68:LYS:HE3	1.91	0.53
1:A:45:TYR:CE2	1:A:67:ALA:HB2	2.44	0.53
2:H:21:ASN:OD1	2:H:22:ILE:N	2.39	0.53
1:D:194:ARG:HB2	1:D:200:THR:HG23	1.90	0.53
1:D:19:GLU:OE1	1:D:75:ARG:HD2	2.08	0.53
1:J:231:VAL:O	1:J:243:LYS:HE2	2.09	0.53
1:D:141:GLN:OE1	1:D:144[A]:ARG:NH1	2.43	0.52
1:D:203:CYS:SG	1:D:272:LEU:HD11	2.49	0.51
1:J:185:PRO:HD2	1:J:266:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:LYS:HD2	3:F:2:CYS:SG	2.50	0.51
1:G:191:HIS:NE2	1:G:199:VAL:HG21	2.25	0.51
1:G:66:LYS:HE3	3:I:2:CYS:SG	2.50	0.51
1:A:192:HIS:HB2	1:A:200:THR:OG1	2.10	0.51
1:D:42:ASN:O	1:D:44:ARG:HG3	2.10	0.51
1:D:44:ARG:NH2	1:D:46:GLU:OE2	2.45	0.50
1:D:63:GLU:OE2	1:D:66:LYS:NZ	2.36	0.50
1:A:163:GLU:O	1:A:167:TRP:N	2.43	0.50
2:K:79:ALA:HB2	2:K:94:TYR:CD2	2.47	0.50
1:J:192:HIS:O	1:J:200:THR:N	2.44	0.50
1:A:41:GLU:CD	1:A:42:ASN:H	2.16	0.49
2:E:36:GLU:OE2	2:E:83:LYS:NZ	2.43	0.49
1:G:226:GLN:O	1:G:227:ASP:OD1	2.29	0.49
1:J:185:PRO:CB	1:J:208:PHE:HB3	2.39	0.49
1:J:55:GLU:HG2	1:J:59:TYR:CD2	2.47	0.49
1:D:191:HIS:CE1	1:D:199:VAL:HG21	2.48	0.49
1:J:21:ARG:NH2	1:J:37:ASP:OD2	2.46	0.49
1:D:202:ARG:HD3	1:D:244:TRP:CD2	2.46	0.48
2:E:89:GLU:HB3	2:E:90:PRO:HD2	1.94	0.48
1:J:81:LEU:HD11	3:L:9:MET:CE	2.42	0.48
2:B:12:ARG:HB3	2:B:22:ILE:HB	1.95	0.48
1:G:44:ARG:HA	1:G:64:THR:HG23	1.94	0.48
1:A:158:ALA:O	1:A:162:GLY:N	2.42	0.48
1:J:183:ASP:O	1:J:208:PHE:HA	2.14	0.48
1:J:107:TRP:O	1:J:169:HIS:NE2	2.34	0.48
1:D:109:LEU:HB2	1:D:165:VAL:HG11	1.95	0.48
1:D:255:GLN:NE2	1:D:274:TRP:O	2.46	0.47
1:J:48:ARG:NH2	2:K:53:ASP:OD2	2.47	0.47
1:A:168:LEU:O	1:A:171:TYR:N	2.46	0.47
1:J:202:ARG:NH2	2:K:98:ASP:O	2.46	0.47
1:G:103:LEU:HD23	1:G:109:LEU:HA	1.97	0.47
1:J:45:TYR:CE2	1:J:67:ALA:HB2	2.48	0.47
1:G:6:ARG:NH2	1:G:113:TYR:CE1	2.83	0.47
1:A:99:SER:HB3	1:A:114:LEU:HD13	1.97	0.47
1:A:268:GLU:OE1	1:D:173:LYS:HE2	2.15	0.47
3:L:6:THR:OG1	3:L:7:ALA:N	2.45	0.47
2:B:34:HIS:CE1	4:B:101:GOL:H12	2.50	0.47
1:D:7:TYR:CE2	3:F:2:CYS:HB3	2.48	0.47
1:G:141:GLN:OE1	1:G:144[A]:ARG:NH1	2.46	0.47
2:K:4:THR:HA	2:K:86:SER:OG	2.14	0.47
2:B:36:GLU:HB2	2:B:83:LYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:40:ALA:O	1:J:43:PRO:HD3	2.15	0.46
1:J:189:VAL:HB	1:J:274:TRP:HA	1.97	0.46
1:D:19:GLU:HA	1:D:19:GLU:OE2	2.16	0.46
1:D:205:ALA:O	1:D:206:LEU:HD23	2.16	0.46
1:D:252:GLY:H	1:D:254:GLU:CD	2.18	0.46
2:E:40:LEU:HD23	2:E:45:LYS:HA	1.98	0.46
2:H:41:LYS:HE3	2:H:78:TYR:OH	2.15	0.46
2:K:21:ASN:HB3	2:K:70:PHE:CE1	2.51	0.46
1:A:99:SER:HA	1:A:113:TYR:O	2.15	0.46
1:G:55:GLU:CD	1:G:170:ARG:HH21	2.19	0.46
1:D:98:MET:HG3	2:E:60:TRP:CZ3	2.50	0.46
1:A:250:PRO:HG2	1:A:253:LYS:HE2	1.98	0.46
2:K:52:SER:HB2	2:K:65:LEU:O	2.16	0.46
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.31	0.45
1:G:81:LEU:HD11	3:I:9:MET:SD	2.56	0.45
1:A:19:GLU:OE1	1:A:75:ARG:NH1	2.50	0.45
1:A:44:ARG:O	1:A:46:GLU:HG2	2.17	0.45
1:G:108:ARG:CZ	1:J:214:THR:HG21	2.46	0.45
1:G:270:LEU:HD23	1:G:270:LEU:HA	1.72	0.45
1:J:73:TRP:CD1	3:L:8:VAL:HG12	2.52	0.45
1:D:163:GLU:OE1	1:D:163:GLU:N	2.39	0.45
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.51	0.45
1:G:209:TYR:CD2	1:G:210:PRO:HA	2.51	0.45
1:G:261:VAL:HB	1:G:270:LEU:HB2	1.99	0.45
1:J:7:TYR:OH	3:L:1:MET:N	2.32	0.45
1:D:252:GLY:N	1:D:254:GLU:OE1	2.50	0.45
1:A:258:THR:HG22	1:A:273:ARG:HG3	1.99	0.45
1:A:107:TRP:CE3	1:A:169:HIS:HD2	2.36	0.44
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.52	0.44
2:B:34:HIS:HE1	4:B:101:GOL:H12	1.83	0.44
2:B:51:MET:SD	2:B:66:ALA:HB2	2.58	0.44
2:K:17:ASN:ND2	2:K:74:GLU:CG	2.80	0.44
1:A:72:GLN:NE2	6:A:302:HOH:O	2.34	0.44
2:B:23:LEU:HB2	2:B:70:PHE:CD1	2.53	0.44
2:H:33:PRO:O	2:H:54[B]:MET:HE1	2.18	0.44
1:J:261:VAL:HB	1:J:270:LEU:HB2	1.97	0.44
2:B:29:GLN:HA	2:B:61:SER:HB2	2.00	0.44
1:A:84:TYR:OH	3:C:9:MET:O	2.22	0.44
1:J:76:VAL:HG22	1:J:79:ARG:NH1	2.33	0.44
1:J:216:THR:OG1	1:J:260:ARG:HB2	2.17	0.44
1:A:152:ALA:HB1	1:A:156:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:219:LEU:HD12	1:J:219:LEU:O	2.16	0.44
1:J:81:LEU:HD11	3:L:9:MET:HE1	1.98	0.43
1:G:264:GLU:HG3	1:G:264:GLU:H	1.59	0.43
1:G:35:ARG:O	1:G:45:TYR:HA	2.18	0.43
1:A:73:TRP:NE1	3:C:8:VAL:HA	2.34	0.43
1:D:191:HIS:NE2	1:D:254:GLU:HG2	2.33	0.43
2:E:49:VAL:HG22	2:E:68:THR:HB	2.00	0.43
1:J:211:ALA:HB1	1:J:233:THR:HG21	2.00	0.43
1:A:49:ALA:HB1	1:A:50:PRO:HD2	2.01	0.43
1:A:81:LEU:HD23	1:A:84:TYR:HD2	1.84	0.43
1:D:201:LEU:CD2	1:D:274:TRP:HB2	2.48	0.43
2:E:38:GLN:OE1	2:E:45:LYS:HG3	2.18	0.43
1:G:5:MET:O	1:G:100:GLY:HA3	2.18	0.42
1:J:102:ASP:O	1:J:110:LEU:N	2.42	0.42
1:J:222:GLU:OE1	1:J:222:GLU:HA	2.19	0.42
1:J:66:LYS:HE3	3:L:2:CYS:SG	2.58	0.42
1:G:52:MET:O	1:G:55:GLU:HG2	2.20	0.42
1:G:19:GLU:OE1	1:G:75:ARG:NE	2.52	0.42
1:A:19:GLU:HA	1:A:19:GLU:OE2	2.19	0.42
1:D:274:TRP:NE1	1:D:276:PRO:HG3	2.34	0.42
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.85	0.42
1:D:201:LEU:HD21	1:D:274:TRP:HB2	2.00	0.42
2:K:56:PHE:HB3	2:K:62:PHE:CD2	2.54	0.42
1:G:55:GLU:CD	1:G:170:ARG:NH2	2.73	0.42
1:D:259:CYS:HB3	1:D:272:LEU:HD12	2.01	0.42
2:B:31:HIS:ND1	6:B:201:HOH:O	2.35	0.42
1:G:97:GLN:HB2	1:G:116:PHE:CE2	2.55	0.42
2:H:41:LYS:HG3	2:H:78:TYR:CE2	2.55	0.42
1:J:147:TRP:CZ2	3:L:9:MET:HG2	2.54	0.42
1:D:185:PRO:HD2	1:D:266:LEU:CD1	2.50	0.42
1:G:11:ALA:HA	1:G:21:ARG:O	2.19	0.41
1:J:147:TRP:O	6:J:302:HOH:O	2.22	0.41
1:D:194:ARG:HD3	1:D:248:VAL:CG2	2.51	0.41
1:A:254:GLU:HB3	1:A:274:TRP:HD1	1.85	0.41
1:G:14:ARG:HB2	1:G:17:LEU:HD13	2.02	0.41
1:D:259:CYS:HB3	1:D:272:LEU:HD11	2.02	0.41
1:D:45:TYR:CE2	1:D:67:ALA:HB2	2.55	0.41
2:E:45:LYS:HE2	2:E:45:LYS:HB2	1.88	0.41
1:D:182:THR:HB	1:D:209:TYR:O	2.20	0.41
1:A:108:ARG:HD3	1:D:262:TYR:CD1	2.56	0.41
1:D:66:LYS:O	1:D:70:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:TRP:CD1	3:I:1:MET:HG2	2.56	0.41
1:G:224:LEU:O	1:G:228:MET:HB2	2.20	0.41
1:G:226:GLN:O	1:G:227:ASP:CB	2.68	0.41
1:J:229:GLU:O	1:J:245:ALA:HA	2.21	0.41
1:J:250:PRO:O	1:J:253:LYS:N	2.54	0.41
1:J:236:ALA:HB1	2:K:12:ARG:HG3	2.02	0.41
1:A:205:ALA:O	1:A:206:LEU:HD23	2.21	0.41
1:D:209:TYR:CG	1:D:210:PRO:HA	2.56	0.41
1:A:129:ASP:O	1:A:131:LYS:HG3	2.20	0.40
2:E:54[B]:MET:CE	2:E:62:PHE:HB3	2.51	0.40
1:J:174:ASN:OD1	1:J:174:ASN:N	2.54	0.40
1:D:192:HIS:HB2	1:D:200:THR:OG1	2.21	0.40
1:J:205:ALA:C	1:J:206:LEU:HD23	2.42	0.40
1:A:119:GLU:CA	1:A:119:GLU:OE1	2.64	0.40
1:D:189:VAL:HG23	1:D:272:LEU:HD13	2.04	0.40
1:D:167:TRP:CD1	3:F:1:MET:HG2	2.56	0.40
1:G:104:GLY:N	1:G:110:LEU:HG	2.37	0.40
1:G:35:ARG:NH2	2:H:53:ASP:HB3	2.36	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:88:ALA:O	1:J:62:ARG:NH1[2_658]	2.16	0.04

## 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	268/276 (97%)	246 (92%)	21 (8%)	1 (0%)	38 42
1	D	269/276 (98%)	257 (96%)	12 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	264/276 (96%)	249 (94%)	15 (6%)	0	100	100
1	J	246/276 (89%)	232 (94%)	11 (4%)	3 (1%)	15	11
2	B	98/99 (99%)	95 (97%)	3 (3%)	0	100	100
2	E	98/99 (99%)	94 (96%)	3 (3%)	1 (1%)	18	15
2	H	98/99 (99%)	95 (97%)	3 (3%)	0	100	100
2	K	98/99 (99%)	92 (94%)	6 (6%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	I	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	L	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	1467/1536 (96%)	1382 (94%)	80 (6%)	5 (0%)	44	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	254	GLU
1	J	251	LEU
1	A	149	GLN
1	J	223	GLU
2	E	47	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	229/234 (98%)	223 (97%)	6 (3%)	51	62
1	D	230/234 (98%)	228 (99%)	2 (1%)	82	89
1	G	226/234 (97%)	223 (99%)	3 (1%)	73	83
1	J	215/234 (92%)	208 (97%)	7 (3%)	43	53
2	B	94/94 (100%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	93/94 (99%)	92 (99%)	1 (1%)	78	86
2	H	94/94 (100%)	93 (99%)	1 (1%)	78	86
2	K	92/94 (98%)	87 (95%)	5 (5%)	26	27
3	C	8/8 (100%)	7 (88%)	1 (12%)	5	3
3	F	8/8 (100%)	8 (100%)	0	100	100
3	I	8/8 (100%)	8 (100%)	0	100	100
3	L	8/8 (100%)	8 (100%)	0	100	100
All	All	1305/1344 (97%)	1279 (98%)	26 (2%)	60	70

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	65	GLN
1	A	115	GLN
1	A	194	ARG
1	A	227	ASP
1	A	230	LEU
3	C	2	CYS
1	D	131	LYS
1	D	183	ASP
2	E	70	PHE
1	G	44	ARG
1	G	272	LEU
1	G	273	ARG
2	H	70	PHE
1	J	92	SER
1	J	192	HIS
1	J	219	LEU
1	J	222	GLU
1	J	253	LYS
1	J	254	GLU
1	J	275	GLU
2	K	17	ASN
2	K	52	SER
2	K	55	SER
2	K	70	PHE
2	K	91	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	70	GLN
1	D	87	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](#)

2 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	GOL	B	101	-	5,5,5	0.34	0	5,5,5	0.30	0
5	SO4	G	301	-	4,4,4	0.19	0	6,6,6	0.13	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
4	GOL	B	101	-	-	0/4/4/4	0/0/0/0
5	SO4	G	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	101	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	272/276 (98%)	0.68	24 (8%) 11 12	23, 48, 89, 106	0
1	D	272/276 (98%)	0.52	26 (9%) 9 9	23, 43, 96, 110	0
1	G	269/276 (97%)	0.52	18 (6%) 19 20	28, 51, 94, 111	0
1	J	258/276 (93%)	0.93	40 (15%) 2 2	24, 62, 115, 145	0
2	B	99/99 (100%)	0.14	1 (1%) 82 84	25, 33, 49, 58	0
2	E	99/99 (100%)	0.26	1 (1%) 82 84	26, 40, 61, 74	0
2	H	99/99 (100%)	0.16	1 (1%) 82 84	30, 41, 56, 73	0
2	K	99/99 (100%)	0.75	7 (7%) 17 18	32, 64, 85, 95	0
3	C	9/9 (100%)	0.38	0 100 100	33, 39, 47, 57	0
3	F	9/9 (100%)	0.02	0 100 100	23, 29, 33, 40	0
3	I	9/9 (100%)	0.17	0 100 100	32, 35, 48, 53	0
3	L	9/9 (100%)	0.28	0 100 100	33, 37, 50, 58	0
All	All	1503/1536 (97%)	0.56	118 (7%) 13 15	23, 47, 93, 145	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	219	LEU	7.3
1	J	224	LEU	6.3
1	J	201	LEU	6.1
1	J	217	TRP	6.0
1	J	251	LEU	5.6
1	J	256	ASN	5.5
1	D	224	LEU	5.5
1	A	224	LEU	5.4
1	J	192	HIS	5.3
1	J	250	PRO	5.3
1	J	252	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	195	SER	5.1
1	J	257	TYR	5.1
1	G	225	THR	5.0
1	G	220	ASN	4.9
1	J	225	THR	4.9
1	D	220	ASN	4.8
1	D	191	HIS	4.7
1	A	225	THR	4.6
1	J	220	ASN	4.6
1	G	224	LEU	4.5
1	J	273	ARG	4.4
1	G	219	LEU	4.4
1	J	200	THR	4.3
1	A	219	LEU	4.2
1	A	197	GLY	4.2
1	A	250	PRO	4.1
1	A	249	VAL	4.0
1	J	255	GLN	3.9
1	J	247	VAL	3.9
1	A	252	GLY	3.8
1	J	253	LYS	3.8
1	D	249	VAL	3.8
1	A	251	LEU	3.8
1	J	258	THR	3.8
1	D	17	LEU	3.8
1	J	274	TRP	3.8
1	J	49	ALA	3.7
1	A	180	LEU	3.7
1	J	16	GLY	3.7
1	G	249	VAL	3.7
1	G	16	GLY	3.5
1	A	61	GLU	3.5
1	A	274	TRP	3.4
1	D	254	GLU	3.4
1	G	217	TRP	3.3
1	A	201	LEU	3.3
1	D	252	GLY	3.3
1	D	225	THR	3.3
2	H	47	PRO	3.3
1	J	270	LEU	3.2
1	J	59	TYR	3.2
1	A	226	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	193	PRO	3.2
1	D	217	TRP	3.1
1	D	201	LEU	3.1
1	J	271	THR	3.0
1	G	227	ASP	2.9
1	J	60	TRP	2.9
1	J	245	ALA	2.9
1	D	273	ARG	2.9
1	A	254	GLU	2.9
1	J	276	PRO	2.9
1	A	191	HIS	2.9
1	G	226	GLN	2.9
1	D	219	LEU	2.9
1	D	226	GLN	2.9
1	A	253	LYS	2.8
2	K	79	ALA	2.8
1	J	44	ARG	2.7
1	D	276	PRO	2.7
1	A	17	LEU	2.7
1	G	17	LEU	2.7
1	G	252	GLY	2.6
2	K	40	LEU	2.6
1	D	199	VAL	2.6
1	J	103	LEU	2.6
1	J	272	LEU	2.5
1	J	223	GLU	2.5
1	J	222	GLU	2.5
1	J	173	LYS	2.5
1	G	248	VAL	2.5
1	D	248	VAL	2.5
1	J	54	GLN	2.5
1	D	181	ARG	2.5
1	G	274	TRP	2.5
1	J	181	ARG	2.5
1	G	256	ASN	2.5
1	D	197	GLY	2.5
1	D	259	CYS	2.4
1	D	207	GLY	2.4
1	A	199	VAL	2.4
2	E	54[A]	MET	2.3
1	G	60	TRP	2.3
1	A	172	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	194	ARG	2.2
2	K	20	PRO	2.2
1	A	181	ARG	2.2
1	J	246	SER	2.2
1	G	197	GLY	2.2
2	K	82	VAL	2.2
1	A	220	ASN	2.2
1	D	223	GLU	2.2
1	D	256	ASN	2.2
2	B	54[A]	MET	2.2
1	G	257	TYR	2.2
1	J	172	LEU	2.1
1	J	213	ILE	2.1
2	K	47	PRO	2.1
1	D	251	LEU	2.1
1	J	167	TRP	2.1
2	K	99	MET	2.1
1	J	190	THR	2.1
1	D	222	GLU	2.0
1	D	227	ASP	2.0
1	A	198	GLU	2.0
1	D	200	THR	2.0
2	K	73	THR	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( $\text{\AA}^2$ )	Q<0.9
5	SO4	G	301	5/5	0.93	0.18	-	75,83,91,92	0
4	GOL	B	101	6/6	0.91	0.12	-	66,69,71,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.