



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:59 AM GMT

PDB ID : 3GSN  
Title : Crystal structure of the public RA14 TCR in complex with the HCMV dominant NLV/HLA-A2 epitope  
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Deposited on : 2009-03-27  
Resolution : 2.80 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

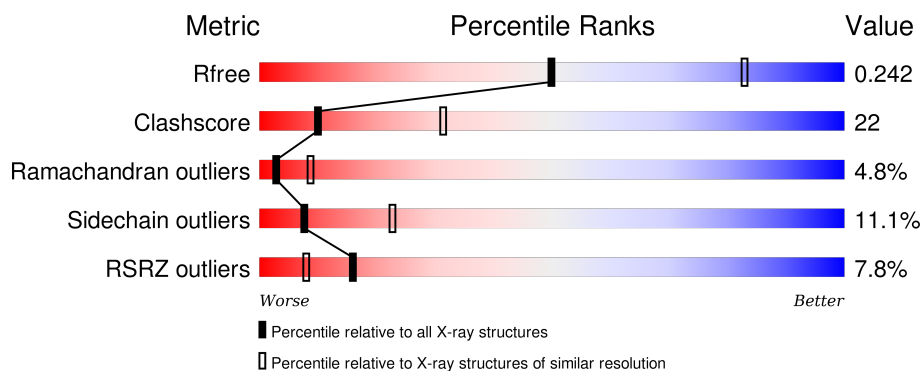
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	H	274	<div> <div>11%</div> <div>61%</div> <div>32%</div> <div>6%</div> </div>
2	P	9	<div> <div>56%</div> <div>44%</div> </div>
3	L	100	<div> <div>5%</div> <div>65%</div> <div>31%</div> <div>•</div> </div>
4	A	199	<div> <div>12%</div> <div>48%</div> <div>40%</div> <div>11%</div> <div>•</div> </div>
5	B	243	<div> <div>2%</div> <div>61%</div> <div>33%</div> <div>6%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6647 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	H	274	Total	C	N	O	S	0	0	0
			2240	1400	408	423	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	245	VAL	ALA	ENGINEERED	UNP P01892

- Molecule 2 is a protein called HCMV pp65 fragment 495-503 (NLVPMVATV).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	9	Total	C	N	O	S	0	0	0
			65	42	10	12	1			

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	INITIATING METHIONINE	UNP P61769

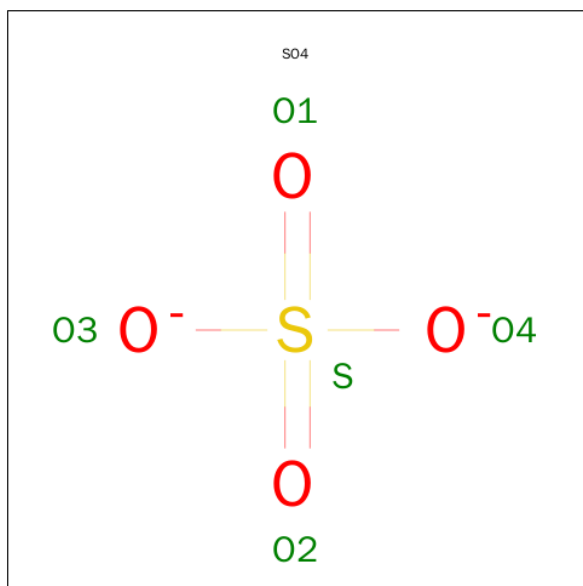
- Molecule 4 is a protein called RA14 TCR alpha chain (TRAV24, TRAJ49).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	199	Total	C	N	O	S	0	0	0
			1567	981	257	322	7			

- Molecule 5 is a protein called RA14 TCR beta chain (TRBV6-5, TRBD1, TRBJ1-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	243	Total	C	N	O	S	0	0	0
			1908	1201	329	368	10			

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



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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

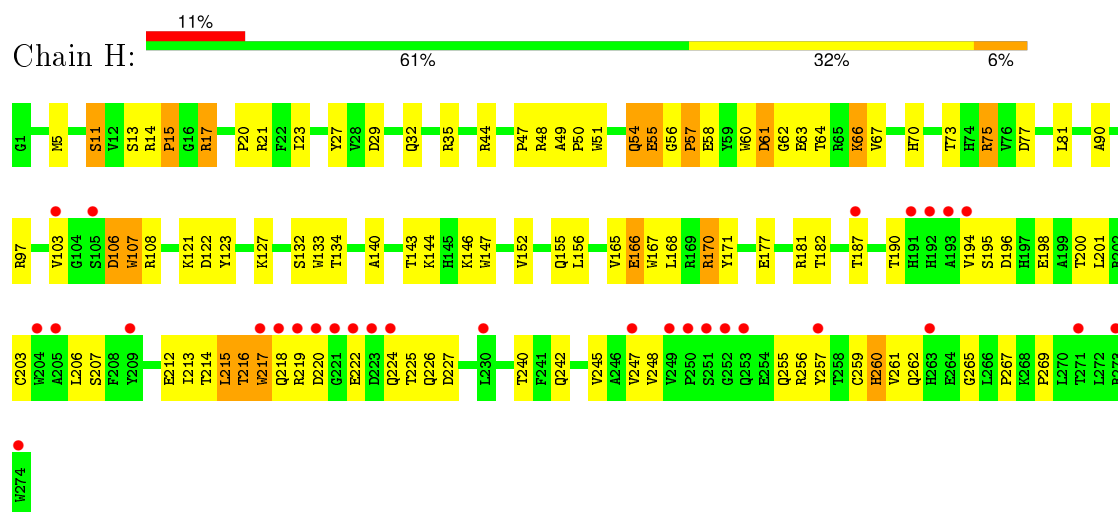
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	5	Total	O	0	0
			5	5		
8	L	6	Total	O	0	0
			6	6		
8	A	4	Total	O	0	0
			4	4		
8	B	9	Total	O	0	0
			9	9		

### 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 errors 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.

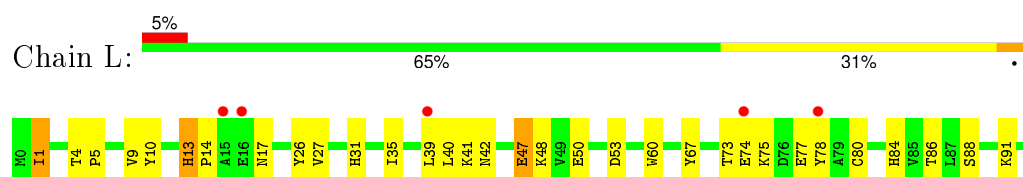
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



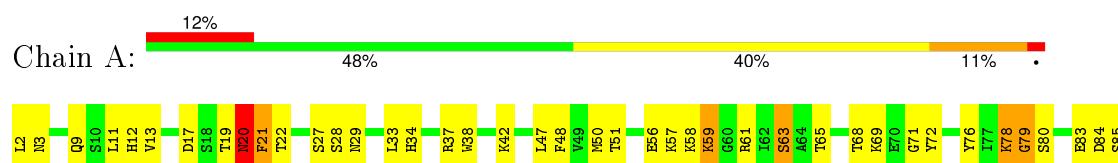
- Molecule 2: HCMV pp65 fragment 495-503 (NLVPMVATV)

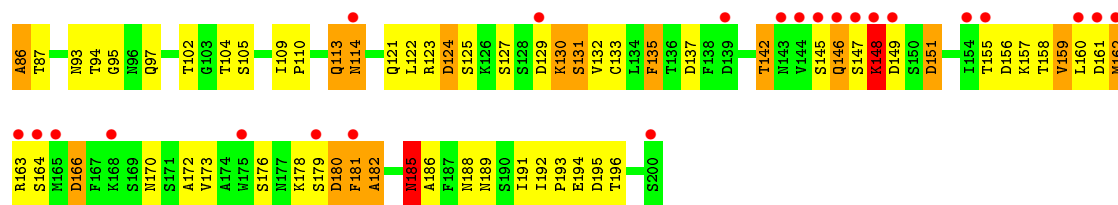


- Molecule 3: Beta-2-microglobulin

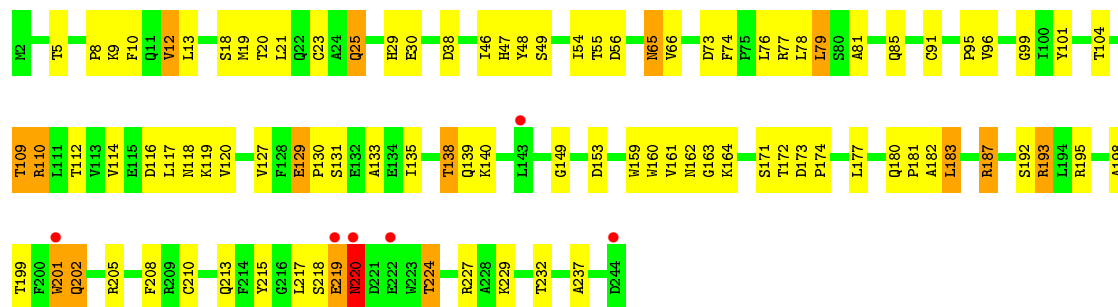


- Molecule 4: RA14 TCR alpha chain (TRAV24, TRAJ49)





- Molecule 5: RA14 TCR beta chain (TRBV6-5, TRBD1, TRBJ1-2)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.45Å 77.06Å 87.22Å 90.00° 101.95° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 42.45 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (15.00-2.80) 94.7 (42.45-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.215 , 0.290 0.237 , 0.242	Depositor DCC
$R_{free}$ test set	2383 reflections (11.58%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 61.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 24045 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4, CL

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	H	0.32	0/2305	0.49	0/3128
2	P	0.43	0/65	0.64	0/88
3	L	0.32	0/860	0.47	0/1162
4	A	0.36	0/1605	0.55	0/2178
5	B	0.35	0/1960	0.50	0/2671
All	All	0.34	0/6795	0.51	0/9227

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2240	0	2094	96	0
2	P	65	0	74	5	0
3	L	837	0	803	41	0
4	A	1567	0	1464	89	0
5	B	1908	0	1812	81	0
6	L	5	0	0	0	0
7	A	1	0	0	0	0
8	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	9	0	0	0	0
8	H	5	0	0	0	0
8	L	6	0	0	1	0
All	All	6647	0	6247	283	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 22.

All (283) 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:H:121:LYS:NZ	3:L:1:ILE:HG12	1.41	1.35
1:H:121:LYS:HE3	3:L:1:ILE:CG1	1.68	1.22
3:L:13:HIS:HB3	3:L:14:PRO:CD	1.73	1.18
1:H:170:ARG:HH11	1:H:170:ARG:HG3	1.00	1.15
1:H:121:LYS:CE	3:L:1:ILE:CG1	2.26	1.12
1:H:121:LYS:CE	3:L:1:ILE:HG13	1.79	1.12
4:A:161:ASP:CB	4:A:162:MET:HA	1.77	1.10
1:H:17:ARG:HG2	1:H:17:ARG:HH11	1.14	1.09
4:A:158:THR:HG23	4:A:170:ASN:HB3	1.11	1.08
3:L:13:HIS:HB3	3:L:14:PRO:HD2	1.33	1.07
4:A:161:ASP:HB3	4:A:162:MET:CA	1.86	1.06
5:B:116:ASP:OD1	5:B:118:ASN:HB2	1.57	1.04
4:A:148:LYS:HB3	4:A:188:ASN:HB2	1.35	1.04
5:B:182:ALA:HA	5:B:183:LEU:HB2	1.35	1.03
1:H:121:LYS:NZ	3:L:1:ILE:CG1	2.23	1.00
1:H:121:LYS:HE3	3:L:1:ILE:HG13	1.00	0.99
3:L:13:HIS:CB	3:L:14:PRO:HD2	1.95	0.96
4:A:161:ASP:HB3	4:A:162:MET:HA	0.96	0.94
1:H:121:LYS:CE	3:L:1:ILE:HG12	1.93	0.94
3:L:13:HIS:CB	3:L:14:PRO:CD	2.46	0.93
1:H:56:GLY:HA2	1:H:60:TRP:HE1	1.34	0.93
4:A:155:THR:HG22	5:B:177:LEU:HD12	1.55	0.88
1:H:170:ARG:HG3	1:H:170:ARG:NH1	1.77	0.87
1:H:121:LYS:HZ2	3:L:1:ILE:HG12	1.04	0.86
4:A:148:LYS:O	4:A:148:LYS:HG3	1.76	0.86
1:H:146:LYS:HE3	5:B:96:VAL:CG1	2.05	0.86
4:A:148:LYS:HE3	4:A:186:ALA:HA	1.57	0.84
5:B:81:ALA:HA	5:B:85:GLN:OE1	1.77	0.84
1:H:219:ARG:HD3	1:H:256:ARG:HD2	1.58	0.83
1:H:17:ARG:CG	1:H:17:ARG:HH11	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:LYS:HE3	5:B:96:VAL:HG12	1.63	0.81
1:H:62:GLY:O	1:H:66:LYS:HG2	1.80	0.81
1:H:106:ASP:O	1:H:107:TRP:HB2	1.78	0.81
4:A:156:ASP:O	4:A:157:LYS:HG3	1.81	0.80
4:A:158:THR:HG23	4:A:170:ASN:CB	2.03	0.80
4:A:38:TRP:NE1	4:A:42:LYS:O	2.15	0.79
1:H:56:GLY:HA2	1:H:60:TRP:NE1	1.98	0.79
4:A:28:SER:O	4:A:29:ASN:HB2	1.82	0.78
4:A:13:VAL:HG11	4:A:19:THR:HG23	1.67	0.76
3:L:13:HIS:HB3	3:L:14:PRO:HD3	1.65	0.76
4:A:158:THR:CG2	4:A:170:ASN:HB3	2.06	0.74
5:B:215:TYR:HA	5:B:232:THR:HG23	1.69	0.74
5:B:182:ALA:HA	5:B:183:LEU:CB	2.08	0.74
4:A:146:GLN:HB3	4:A:149:ASP:OD1	1.88	0.74
3:L:17:ASN:HD21	3:L:74:GLU:HB3	1.52	0.73
5:B:129:GLU:HG3	5:B:201:TRP:CH2	2.24	0.73
5:B:202:GLN:HE21	5:B:202:GLN:HA	1.54	0.72
4:A:124:ASP:CG	4:A:125:SER:H	1.92	0.72
1:H:170:ARG:HH11	1:H:170:ARG:CG	1.91	0.72
4:A:157:LYS:HE2	5:B:174:PRO:HD2	1.73	0.71
1:H:17:ARG:NH1	1:H:17:ARG:HG2	1.95	0.71
5:B:182:ALA:CA	5:B:183:LEU:HB2	2.18	0.71
4:A:110:PRO:CD	4:A:158:THR:HG21	2.22	0.69
4:A:93:ASN:HA	4:A:97:GLN:O	1.93	0.69
4:A:148:LYS:CB	4:A:188:ASN:HB2	2.18	0.69
5:B:65:ASN:C	5:B:65:ASN:HD22	1.96	0.68
4:A:129:ASP:O	4:A:131:SER:N	2.25	0.68
5:B:21:LEU:HB2	5:B:76:LEU:HB3	1.75	0.68
4:A:61:ARG:HD2	4:A:79:GLY:O	1.93	0.67
4:A:135:PHE:HB3	4:A:172:ALA:HB3	1.76	0.67
1:H:56:GLY:N	1:H:57:PRO:HD3	2.09	0.67
4:A:110:PRO:HD2	4:A:158:THR:HG21	1.77	0.67
1:H:73:THR:HG21	2:P:6:VAL:HG12	1.76	0.66
3:L:17:ASN:ND2	3:L:74:GLU:HB3	2.10	0.66
1:H:219:ARG:HB2	1:H:257:TYR:CE1	2.30	0.66
5:B:224:THR:OG1	5:B:224:THR:O	2.12	0.65
5:B:46:ILE:HG22	5:B:47:HIS:HD2	1.58	0.65
4:A:151:ASP:O	4:A:176:SER:OG	2.14	0.65
1:H:146:LYS:HE3	5:B:96:VAL:HG11	1.77	0.65
1:H:55:GLU:C	1:H:57:PRO:HD3	2.17	0.65
4:A:148:LYS:HZ1	4:A:181:PHE:HE1	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:192:ILE:HD12	4:A:196:THR:HG21	1.79	0.65
4:A:85:SER:O	4:A:86:ALA:HB2	1.97	0.64
3:L:17:ASN:HD21	3:L:74:GLU:CB	2.11	0.63
1:H:200:THR:O	1:H:201:LEU:HB2	1.98	0.63
4:A:56:GLU:HG3	4:A:65:THR:HG22	1.79	0.63
4:A:192:ILE:HB	4:A:193:PRO:HD2	1.81	0.63
4:A:181:PHE:O	4:A:182:ALA:HB3	1.98	0.63
5:B:116:ASP:OD1	5:B:118:ASN:CB	2.41	0.62
1:H:5:MET:HB2	1:H:168:LEU:HD13	1.81	0.62
4:A:27:SER:HB2	4:A:68:THR:O	1.99	0.62
1:H:61:ASP:O	1:H:64:THR:HG22	2.00	0.62
1:H:219:ARG:CD	1:H:256:ARG:HD2	2.30	0.61
1:H:49:ALA:HB1	1:H:51:TRP:NE1	2.16	0.60
5:B:202:GLN:NE2	5:B:202:GLN:HA	2.17	0.59
1:H:47:PRO:O	1:H:48:ARG:NH2	2.34	0.59
1:H:219:ARG:O	1:H:220:ASP:HB3	2.01	0.59
4:A:20:ASN:HB2	4:A:76:TYR:CD1	2.36	0.59
1:H:121:LYS:HZ1	3:L:1:ILE:HG12	1.56	0.59
5:B:65:ASN:HD21	5:B:77:ARG:HB3	1.67	0.59
1:H:217:TRP:HE1	1:H:245:VAL:HG22	1.66	0.58
5:B:120:VAL:O	5:B:227:ARG:NH2	2.32	0.57
5:B:65:ASN:ND2	5:B:77:ARG:HB3	2.19	0.57
5:B:161:VAL:C	5:B:163:GLY:H	2.08	0.57
4:A:142:THR:HG23	4:A:191:ILE:HG22	1.86	0.57
1:H:170:ARG:CG	1:H:170:ARG:NH1	2.58	0.56
3:L:94:LYS:H	3:L:94:LYS:HD3	1.71	0.56
4:A:178:LYS:O	4:A:179:SER:HB3	2.06	0.56
1:H:214:THR:O	1:H:261:VAL:HA	2.05	0.56
1:H:194:VAL:HG22	1:H:198:GLU:O	2.07	0.55
1:H:206:LEU:HG	1:H:242:GLN:HG2	1.87	0.55
4:A:110:PRO:HD2	4:A:158:THR:CG2	2.36	0.55
4:A:110:PRO:HD3	4:A:158:THR:HG21	1.87	0.55
5:B:129:GLU:CG	5:B:201:TRP:CH2	2.89	0.55
4:A:147:SER:HA	4:A:189:ASN:HB3	1.88	0.55
1:H:13:SER:C	1:H:14:ARG:HG3	2.27	0.55
1:H:190:THR:O	1:H:201:LEU:HA	2.07	0.55
4:A:87:THR:HA	4:A:105:SER:HA	1.88	0.55
4:A:21:PHE:CD1	4:A:21:PHE:N	2.70	0.54
3:L:50:GLU:OE2	3:L:67:TYR:CE1	2.60	0.54
1:H:203:CYS:HB2	1:H:217:TRP:CH2	2.43	0.54
4:A:110:PRO:CD	4:A:158:THR:CG2	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:78:TYR:HB2	3:L:95:TRP:HE3	1.72	0.54
5:B:220:ASN:C	5:B:220:ASN:HD22	2.11	0.54
4:A:129:ASP:C	4:A:131:SER:H	2.08	0.54
1:H:227:ASP:HB3	1:H:248:VAL:HG23	1.90	0.53
4:A:13:VAL:HG11	4:A:19:THR:CG2	2.37	0.53
5:B:96:VAL:HG22	5:B:101:TYR:CD2	2.44	0.53
3:L:50:GLU:OE2	3:L:67:TYR:HE1	1.91	0.53
5:B:192:SER:HA	5:B:193:ARG:NH1	2.24	0.53
1:H:127:LYS:HE3	1:H:134:THR:OG1	2.08	0.53
1:H:219:ARG:HD3	1:H:256:ARG:CD	2.36	0.53
1:H:212:GLU:HA	1:H:212:GLU:OE2	2.09	0.52
4:A:95:GLY:H	4:A:97:GLN:HB2	1.74	0.52
1:H:32:GLN:HE22	3:L:53:ASP:HB2	1.74	0.52
4:A:130:LYS:O	4:A:131:SER:C	2.47	0.52
1:H:216:THR:HG22	1:H:217:TRP:H	1.73	0.52
4:A:113:GLN:O	4:A:114:ASN:C	2.48	0.52
3:L:13:HIS:HB2	3:L:14:PRO:HD2	1.87	0.52
3:L:39:LEU:O	3:L:40:LEU:HD23	2.09	0.52
4:A:181:PHE:O	4:A:182:ALA:CB	2.57	0.52
4:A:56:GLU:CG	4:A:65:THR:HG22	2.40	0.52
5:B:49:SER:HB2	5:B:74:PHE:CE1	2.45	0.52
3:L:47:GLU:HG2	3:L:48:LYS:N	2.25	0.52
4:A:58:LYS:HA	4:A:63:SER:HA	1.92	0.52
5:B:8:PRO:O	5:B:109:THR:HB	2.10	0.52
4:A:157:LYS:CE	5:B:174:PRO:HD2	2.40	0.51
1:H:75:ARG:HH12	5:B:54:ILE:HG23	1.75	0.51
1:H:11:SER:HA	1:H:21:ARG:O	2.10	0.51
4:A:56:GLU:CD	4:A:65:THR:HG22	2.31	0.51
5:B:161:VAL:O	5:B:163:GLY:N	2.43	0.51
5:B:96:VAL:HG23	5:B:99:GLY:HA3	1.92	0.51
4:A:124:ASP:CG	4:A:125:SER:N	2.62	0.51
4:A:17:ASP:O	4:A:80:SER:OG	2.24	0.51
5:B:116:ASP:OD1	5:B:118:ASN:N	2.41	0.50
4:A:50:MET:SD	4:A:57:LYS:HG2	2.50	0.50
5:B:140:LYS:HZ2	5:B:195:ARG:NH2	2.10	0.50
5:B:110:ARG:NH2	5:B:153:ASP:OD2	2.44	0.50
1:H:213:ILE:HG13	1:H:262:GLN:O	2.11	0.50
1:H:56:GLY:HA2	1:H:60:TRP:CD1	2.47	0.50
4:A:161:ASP:CB	4:A:162:MET:CA	2.65	0.50
4:A:20:ASN:CB	4:A:76:TYR:CD1	2.95	0.50
3:L:40:LEU:O	3:L:78:TYR:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:ASP:O	1:H:107:TRP:CB	2.51	0.50
5:B:140:LYS:NZ	5:B:195:ARG:NH2	2.59	0.50
3:L:94:LYS:HD3	3:L:94:LYS:N	2.27	0.49
4:A:148:LYS:HB3	4:A:188:ASN:CB	2.25	0.49
5:B:46:ILE:HG22	5:B:47:HIS:CD2	2.44	0.49
1:H:224:GLN:O	1:H:226:GLN:N	2.45	0.49
1:H:123:TYR:O	1:H:140:ALA:HB1	2.11	0.49
5:B:131:SER:C	5:B:133:ALA:H	2.15	0.49
5:B:149:GLY:HA2	5:B:187:ARG:HB3	1.95	0.49
5:B:117:LEU:HD22	5:B:217:LEU:HD21	1.95	0.49
1:H:217:TRP:NE1	1:H:245:VAL:HG22	2.27	0.49
5:B:78:LEU:O	5:B:79:LEU:C	2.51	0.48
4:A:156:ASP:C	4:A:157:LYS:HG3	2.33	0.48
5:B:135:ILE:HG23	5:B:198:ALA:HB1	1.95	0.48
5:B:180:GLN:O	5:B:182:ALA:N	2.47	0.48
1:H:51:TRP:CZ3	1:H:171:TYR:HB3	2.48	0.48
4:A:11:LEU:HD11	4:A:19:THR:HG21	1.95	0.47
3:L:35:ILE:HG23	3:L:35:ILE:O	2.14	0.47
1:H:51:TRP:HZ3	1:H:171:TYR:HB3	1.78	0.47
5:B:180:GLN:C	5:B:182:ALA:H	2.18	0.47
5:B:65:ASN:C	5:B:65:ASN:ND2	2.67	0.47
3:L:5:PRO:HB3	3:L:27:VAL:CG2	2.44	0.47
1:H:227:ASP:HB3	1:H:248:VAL:CG2	2.44	0.47
5:B:25:GLN:NE2	5:B:29:HIS:HB2	2.29	0.47
1:H:219:ARG:CG	1:H:256:ARG:HD2	2.45	0.47
4:A:178:LYS:O	4:A:179:SER:CB	2.63	0.47
1:H:247:VAL:HG22	1:H:248:VAL:N	2.29	0.47
1:H:66:LYS:NZ	2:P:2:LEU:O	2.48	0.46
4:A:11:LEU:CD1	4:A:19:THR:HG21	2.45	0.46
5:B:12:VAL:O	5:B:13:LEU:HD23	2.15	0.46
1:H:123:TYR:O	1:H:140:ALA:CB	2.63	0.46
5:B:96:VAL:HG22	5:B:101:TYR:HD2	1.80	0.46
1:H:207:SER:HA	1:H:240:THR:HB	1.97	0.46
3:L:42:ASN:HA	3:L:77:GLU:HB2	1.98	0.46
5:B:201:TRP:HE3	5:B:208:PHE:CE2	2.34	0.46
1:H:146:LYS:CE	5:B:96:VAL:HG12	2.38	0.46
1:H:143:THR:O	1:H:147:TRP:HB2	2.16	0.46
5:B:9:LYS:HB2	5:B:10:PHE:CD2	2.51	0.46
4:A:83:GLU:CD	4:A:83:GLU:H	2.19	0.46
3:L:41:LYS:NZ	8:L:105:HOH:O	2.49	0.46
1:H:63:GLU:OE1	1:H:66:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:GLN:O	1:H:55:GLU:HB2	2.16	0.45
1:H:103:VAL:HG13	1:H:168:LEU:HD23	1.98	0.45
5:B:66:VAL:HG12	5:B:76:LEU:HA	1.98	0.45
1:H:216:THR:O	1:H:259:CYS:HA	2.17	0.45
4:A:191:ILE:O	4:A:191:ILE:HG23	2.16	0.45
1:H:152:VAL:O	1:H:156:LEU:HG	2.16	0.45
1:H:106:ASP:N	1:H:106:ASP:OD2	2.37	0.45
4:A:162:MET:HB2	4:A:163:ARG:H	1.48	0.45
4:A:85:SER:O	4:A:86:ALA:CB	2.62	0.45
4:A:20:ASN:CG	4:A:20:ASN:O	2.55	0.45
5:B:193:ARG:HH11	5:B:193:ARG:N	2.15	0.45
5:B:140:LYS:HD3	5:B:195:ARG:NE	2.32	0.45
4:A:2:LEU:HD12	4:A:3:ASN:N	2.32	0.45
1:H:14:ARG:HB3	1:H:17:ARG:HD3	1.99	0.44
1:H:121:LYS:HZ1	3:L:1:ILE:CG1	2.21	0.44
4:A:185:ASN:HD22	4:A:185:ASN:HA	1.62	0.44
4:A:48:PHE:HE1	4:A:59:LYS:HB3	1.82	0.44
4:A:58:LYS:HB2	4:A:63:SER:HB3	2.00	0.44
5:B:139:GLN:C	5:B:198:ALA:HB2	2.37	0.44
5:B:13:LEU:HD11	5:B:19:MET:HE2	1.99	0.44
4:A:135:PHE:HE2	4:A:192:ILE:HG21	1.81	0.44
5:B:205:ARG:HA	5:B:205:ARG:HD2	1.85	0.44
3:L:9:VAL:CG1	3:L:95:TRP:HB2	2.47	0.44
5:B:116:ASP:C	5:B:118:ASN:N	2.70	0.44
1:H:218:GLN:O	1:H:257:TYR:HA	2.18	0.44
4:A:61:ARG:NH1	4:A:84:ASP:OD2	2.37	0.44
4:A:137:ASP:OD1	4:A:137:ASP:N	2.51	0.44
4:A:33:LEU:C	4:A:34:HIS:HD2	2.22	0.43
1:H:220:ASP:C	1:H:222:GLU:H	2.21	0.43
5:B:130:PRO:HD2	5:B:201:TRP:CZ2	2.54	0.43
5:B:110:ARG:HB3	5:B:110:ARG:HE	1.48	0.43
1:H:70:HIS:NE2	2:P:3:VAL:HG12	2.34	0.43
1:H:97:ARG:NH1	2:P:6:VAL:HG11	2.34	0.43
4:A:159:VAL:HB	5:B:171:SER:HB2	2.00	0.43
3:L:84:HIS:CE1	3:L:86:THR:HG23	2.54	0.43
5:B:218:SER:O	5:B:220:ASN:N	2.51	0.43
5:B:192:SER:CA	5:B:193:ARG:NH1	2.82	0.43
5:B:114:VAL:HB	5:B:119:LYS:HD2	2.00	0.43
4:A:121:GLN:C	4:A:122:LEU:HD12	2.39	0.43
5:B:127:VAL:HG23	5:B:237:ALA:HB3	2.01	0.42
5:B:30:GLU:HG3	5:B:95:PRO:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:ARG:CZ	2:P:6:VAL:HG11	2.48	0.42
1:H:133:TRP:HB2	1:H:144:LYS:HG3	2.01	0.42
4:A:132:VAL:HG13	4:A:173:VAL:HG23	2.01	0.42
1:H:215:LEU:HA	1:H:260:HIS:O	2.18	0.42
5:B:138:THR:O	5:B:139:GLN:HB2	2.19	0.42
1:H:165:VAL:O	1:H:167:TRP:N	2.53	0.42
4:A:178:LYS:C	4:A:180:ASP:H	2.22	0.42
1:H:220:ASP:O	1:H:220:ASP:CG	2.57	0.42
3:L:9:VAL:HG11	3:L:95:TRP:HB2	2.02	0.42
5:B:18:SER:HB3	5:B:79:LEU:O	2.19	0.41
3:L:4:THR:HA	3:L:5:PRO:HD3	1.91	0.41
3:L:10:TYR:OH	3:L:26:TYR:HB2	2.19	0.41
5:B:172:THR:HG22	5:B:173:ASP:H	1.84	0.41
1:H:60:TRP:O	1:H:64:THR:HB	2.19	0.41
4:A:50:MET:SD	4:A:57:LYS:CG	3.08	0.41
4:A:166:ASP:O	5:B:195:ARG:NH2	2.53	0.41
3:L:4:THR:HG22	3:L:5:PRO:HD2	2.03	0.41
3:L:73:THR:C	3:L:75:LYS:H	2.23	0.41
1:H:195:SER:HB2	1:H:196:ASP:H	1.68	0.41
1:H:64:THR:O	1:H:67:VAL:HG12	2.20	0.41
4:A:178:LYS:HB3	4:A:180:ASP:OD2	2.21	0.41
1:H:17:ARG:CG	1:H:17:ARG:NH1	2.60	0.41
5:B:129:GLU:HG3	5:B:201:TRP:HH2	1.79	0.41
3:L:78:TYR:HB2	3:L:95:TRP:CE3	2.55	0.41
4:A:2:LEU:HD12	4:A:3:ASN:H	1.86	0.41
1:H:122:ASP:OD1	3:L:60:TRP:NE1	2.37	0.41
4:A:109:ILE:HA	4:A:110:PRO:HD3	1.86	0.41
1:H:81:LEU:HD21	1:H:123:TYR:CZ	2.56	0.41
4:A:78:LYS:O	4:A:79:GLY:C	2.57	0.41
1:H:27:TYR:CZ	1:H:32:GLN:HB2	2.56	0.41
5:B:159:TRP:HA	5:B:210:CYS:HA	2.02	0.41
5:B:161:VAL:C	5:B:163:GLY:N	2.74	0.41
1:H:75:ARG:NH1	5:B:54:ILE:HG23	2.35	0.41
5:B:159:TRP:C	5:B:160:TRP:CD1	2.94	0.41
5:B:48:TYR:CZ	5:B:56:ASP:HB3	2.56	0.41
4:A:12:HIS:HB3	4:A:109:ILE:HD11	2.03	0.41
4:A:38:TRP:CD1	4:A:42:LYS:O	2.74	0.41
1:H:49:ALA:HB1	1:H:51:TRP:HE1	1.83	0.41
1:H:44:ARG:HH11	1:H:64:THR:HG21	1.86	0.41
5:B:19:MET:HG2	5:B:20:THR:N	2.36	0.41
4:A:72:TYR:CD2	4:A:72:TYR:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:159:TRP:O	5:B:160:TRP:CD1	2.75	0.40
1:H:13:SER:HA	1:H:20:PRO:HB3	2.02	0.40
1:H:14:ARG:HA	1:H:15:PRO:HD2	1.79	0.40
5:B:172:THR:HG22	5:B:173:ASP:N	2.36	0.40
4:A:69:LYS:HD3	4:A:69:LYS:HA	1.82	0.40
5:B:219:GLU:HA	5:B:229:LYS:NZ	2.36	0.40
1:H:155:GLN:HE22	4:A:51:THR:HB	1.87	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	H	272/274 (99%)	223 (82%)	35 (13%)	14 (5%)	2	8
2	P	7/9 (78%)	7 (100%)	0	0	100	100
3	L	98/100 (98%)	89 (91%)	7 (7%)	2 (2%)	9	30
4	A	197/199 (99%)	149 (76%)	31 (16%)	17 (9%)	1	2
5	B	241/243 (99%)	219 (91%)	16 (7%)	6 (2%)	7	24
All	All	815/825 (99%)	687 (84%)	89 (11%)	39 (5%)	3	9

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	55	GLU
1	H	57	PRO
1	H	90	ALA
1	H	225	THR
3	L	13	HIS
3	L	47	GLU
4	A	124	ASP

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Mol	Chain	Res	Type
4	A	130	LYS
4	A	185	ASN
1	H	15	PRO
1	H	107	TRP
1	H	267	PRO
4	A	71	GLY
4	A	131	SER
4	A	182	ALA
5	B	219	GLU
5	B	220	ASN
1	H	29	ASP
1	H	50	PRO
1	H	166	GLU
1	H	269	PRO
4	A	20	ASN
4	A	78	LYS
4	A	86	ALA
4	A	166	ASP
5	B	162	ASN
1	H	77	ASP
1	H	255	GLN
4	A	127	SER
4	A	148	LYS
4	A	164	SER
4	A	181	PHE
5	B	79	LEU
5	B	181	PRO
5	B	183	LEU
4	A	145	SER
4	A	79	GLY
4	A	114	ASN
1	H	265	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	231/231 (100%)	209 (90%)	22 (10%)	11	30
2	P	8/8 (100%)	7 (88%)	1 (12%)	6	17
3	L	95/95 (100%)	88 (93%)	7 (7%)	17	43
4	A	178/178 (100%)	152 (85%)	26 (15%)	4	11
5	B	210/210 (100%)	186 (89%)	24 (11%)	7	21
All	All	722/722 (100%)	642 (89%)	80 (11%)	8	23

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	SER
1	H	17	ARG
1	H	23	ILE
1	H	35	ARG
1	H	54	GLN
1	H	58	GLU
1	H	61	ASP
1	H	66	LYS
1	H	75	ARG
1	H	106	ASP
1	H	108	ARG
1	H	132	SER
1	H	166	GLU
1	H	170	ARG
1	H	177	GLU
1	H	181	ARG
1	H	182	THR
1	H	187	THR
1	H	215	LEU
1	H	216	THR
1	H	217	TRP
1	H	260	HIS
2	P	8	THR
3	L	1	ILE
3	L	31	HIS
3	L	80	CYS
3	L	88	SER
3	L	91	LYS
3	L	94	LYS
3	L	99	MET
4	A	9	GLN

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Mol	Chain	Res	Type
4	A	20	ASN
4	A	21	PHE
4	A	22	THR
4	A	37	ARG
4	A	47	LEU
4	A	59	LYS
4	A	63	SER
4	A	94	THR
4	A	102	THR
4	A	104	THR
4	A	113	GLN
4	A	123	ARG
4	A	133	CYS
4	A	135	PHE
4	A	142	THR
4	A	146	GLN
4	A	148	LYS
4	A	151	ASP
4	A	159	VAL
4	A	160	LEU
4	A	162	MET
4	A	180	ASP
4	A	185	ASN
4	A	194	GLU
4	A	195	ASP
5	B	5	THR
5	B	12	VAL
5	B	23	CYS
5	B	25	GLN
5	B	38	ASP
5	B	55	THR
5	B	65	ASN
5	B	73	ASP
5	B	91	CYS
5	B	104	THR
5	B	109	THR
5	B	110	ARG
5	B	112	THR
5	B	129	GLU
5	B	138	THR
5	B	164	LYS
5	B	187	ARG

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Mol	Chain	Res	Type
5	B	193	ARG
5	B	199	THR
5	B	201	TRP
5	B	202	GLN
5	B	213	GLN
5	B	220	ASN
5	B	224	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	32	GLN
1	H	114	HIS
1	H	155	GLN
1	H	174	ASN
1	H	224	GLN
4	A	9	GLN
4	A	12	HIS
4	A	20	ASN
4	A	34	HIS
4	A	81	GLN
4	A	114	ASN
4	A	143	ASN
4	A	185	ASN
4	A	188	ASN
5	B	17	GLN
5	B	22	GLN
5	B	25	GLN
5	B	47	HIS
5	B	65	ASN
5	B	118	ASN
5	B	175	GLN
5	B	202	GLN
5	B	206	ASN
5	B	213	GLN
5	B	220	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	L	800	-	4,4,4	0.12	0	6,6,6	0.14	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	L	800	-	-	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.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	H	274/274 (100%)	0.67	30 (10%) <b>7</b> <b>3</b>	31, 49, 76, 78	25 (9%)
2	P	9/9 (100%)	0.26	0 <b>100</b> <b>100</b>	35, 36, 40, 40	0
3	L	100/100 (100%)	0.37	5 (5%) <b>32</b> <b>21</b>	35, 50, 68, 70	10 (10%)
4	A	199/199 (100%)	0.65	23 (11%) <b>6</b> <b>3</b>	35, 51, 79, 85	18 (9%)
5	B	243/243 (100%)	0.25	6 (2%) <b>61</b> <b>48</b>	30, 49, 67, 70	0
All	All	825/825 (100%)	0.50	64 (7%) <b>16</b> <b>8</b>	30, 50, 76, 85	53 (6%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	252	GLY	8.9
4	A	149	ASP	7.9
4	A	163	ARG	7.5
1	H	222	GLU	6.5
4	A	160	LEU	5.8
4	A	146	GLN	5.1
4	A	165	MET	4.9
4	A	162	MET	4.8
4	A	161	ASP	4.6
1	H	223	ASP	4.5
1	H	251	SER	4.0
1	H	253	GLN	3.8
1	H	220	ASP	3.8
4	A	147	SER	3.6
4	A	168	LYS	3.5
1	H	250	PRO	3.4
1	H	219	ARG	3.4
1	H	205	ALA	3.3
3	L	15	ALA	3.2
3	L	16	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	209	TYR	3.0
1	H	257	TYR	3.0
1	H	217	TRP	3.0
4	A	200	SER	2.9
1	H	249	VAL	2.9
3	L	74	GLU	2.9
4	A	164	SER	2.9
1	H	192	HIS	2.9
5	B	244	ASP	2.8
4	A	155	THR	2.8
1	H	187	THR	2.8
1	H	273	ARG	2.8
4	A	154	ILE	2.7
1	H	103	VAL	2.7
4	A	114	ASN	2.7
1	H	105	SER	2.6
4	A	145	SER	2.6
1	H	274	TRP	2.6
4	A	144	VAL	2.6
1	H	221	GLY	2.5
5	B	201	TRP	2.5
1	H	191	HIS	2.4
1	H	247	VAL	2.4
4	A	139	ASP	2.3
1	H	230	LEU	2.3
4	A	179	SER	2.2
1	H	194	VAL	2.2
4	A	143	ASN	2.2
5	B	220	ASN	2.2
4	A	148	LYS	2.2
5	B	222	GLU	2.2
5	B	143	LEU	2.1
1	H	218	GLN	2.1
1	H	224	GLN	2.1
1	H	263	HIS	2.1
3	L	78	TYR	2.1
4	A	129	ASP	2.1
1	H	193	ALA	2.1
1	H	271	THR	2.0
3	L	39	LEU	2.0
4	A	181	PHE	2.0
4	A	175	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
5	B	219	GLU	2.0
1	H	204	TRP	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
7	CL	A	1	1/1	0.89	0.14	-1.16	53,53,53,53	0
6	SO4	L	800	5/5	0.92	0.14	-	78,78,79,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.