



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:14 AM GMT

PDB ID : 3LD8  
Title : Structure of JMJD6 and Fab Fragments  
Authors : Hong, X.; Zang, J.; White, J.; Kappler, J.W.; Wang, C.; Zhang, G.  
Deposited on : 2010-01-12  
Resolution : 2.70 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

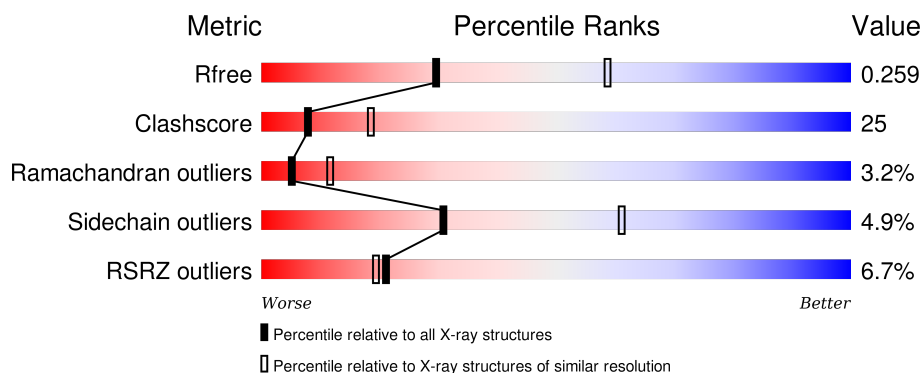
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	334	<div> <div>10%</div> <div>63% 33% .</div> </div>
2	B	220	<div> <div>10%</div> <div>49% 43% 6% ..</div> </div>
3	C	221	<div> <div>11%</div> <div>56% 34% 5% 5%</div> </div>

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
5	GOL	A	337	-	-	-	X
5	GOL	A	339	-	-	-	X
6	SO4	A	341	-	-	-	X
6	SO4	A	348	-	-	X	-
6	SO4	B	223	-	-	-	X
6	SO4	C	223	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6201 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 Bifunctional arginine demethylase and lysyl-hydroxylase JMJD6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2789	1788	492	502	7			

- Molecule 2 is a protein called antibody Fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1666	1048	275	336	7			

- Molecule 3 is a protein called antibody Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	210	Total	C	N	O	S	0	0	0
			1618	1029	265	318	6			

- Molecule 4 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Hg	0	0
			2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

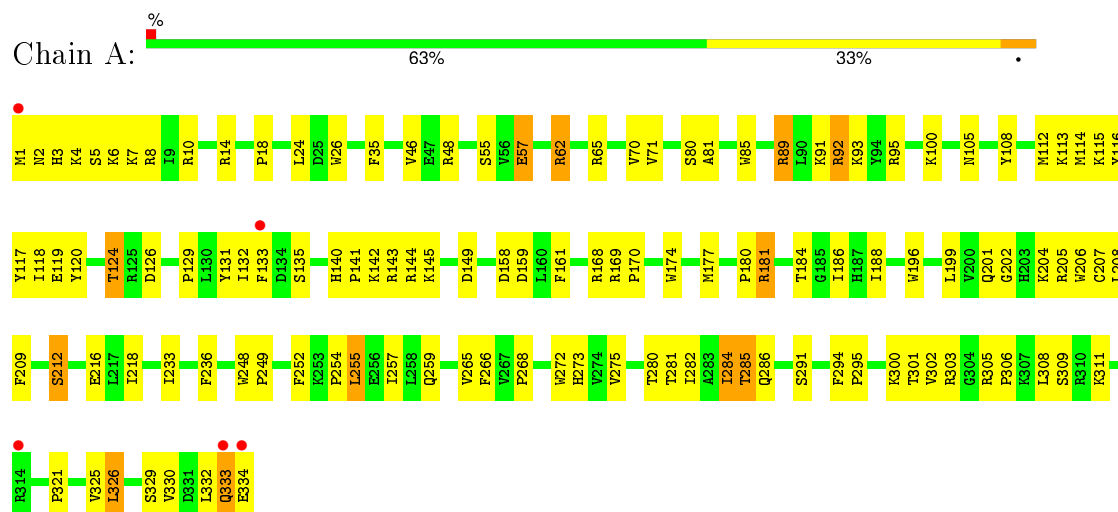
- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

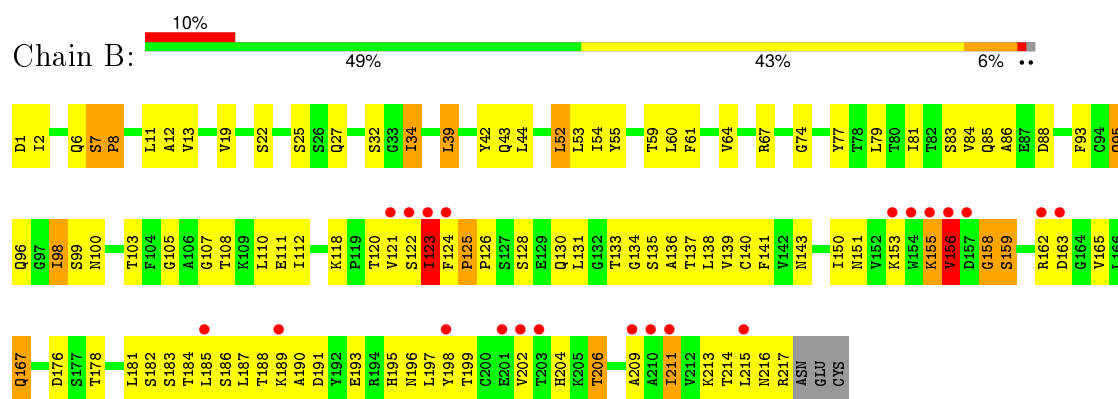
### 3 Residue-property plots

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.

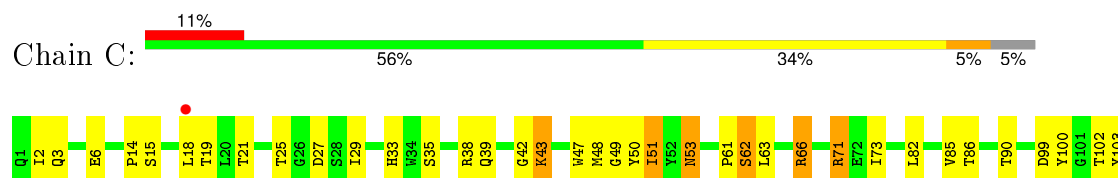
- Molecule 1: Bifunctional arginine demethylase and lysyl-hydroxylase JMJD6

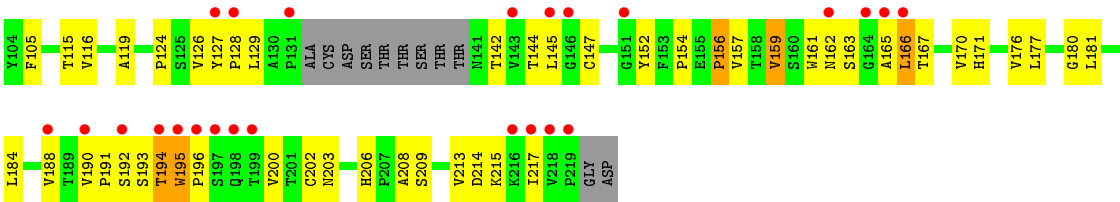


- Molecule 2: antibody Fab fragment light chain



- Molecule 3: antibody Fab fragment heavy chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.28Å 138.28Å 183.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.89 – 2.70 48.89 – 2.61	Depositor EDS
% Data completeness (in resolution range)	74.4 (48.89-2.70) 67.9 (48.89-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.92 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.233 , 0.260 0.233 , 0.259	Depositor DCC
$R_{free}$ test set	943 reflections (2.56%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 40942 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6201	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG, GOL, SO4, FE

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	0.39	0/2874	0.66	1/3896 (0.0%)
2	B	0.44	1/1699 (0.1%)	0.78	3/2304 (0.1%)
3	C	0.44	0/1664	0.71	1/2282 (0.0%)
All	All	0.42	1/6237 (0.0%)	0.71	5/8482 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	209	ALA	CA-CB	5.35	1.63	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	GLY	N-CA-C	10.75	139.98	113.10
2	B	159	SER	CB-CA-C	10.42	129.90	110.10
1	A	181	ARG	CB-CA-C	-8.24	93.91	110.40
2	B	123	ILE	CB-CA-C	-8.24	95.12	111.60
3	C	42	GLY	N-CA-C	-5.53	99.27	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	155	LYS	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2789	0	2739	102	0
2	B	1666	0	1644	131	0
3	C	1618	0	1568	81	0
4	A	2	0	0	0	0
5	A	24	0	32	4	0
5	B	6	0	8	0	0
6	A	70	0	0	3	0
6	B	10	0	0	0	0
6	C	15	0	0	0	0
7	A	1	0	0	0	0
All	All	6201	0	5991	303	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 25.

All (303) 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)
2:B:158:GLY:O	2:B:159:SER:OG	1.69	1.11
2:B:155:LYS:HB3	2:B:156:VAL:O	1.51	1.10
2:B:125:PRO:HA	2:B:138:LEU:HD23	1.36	1.04
2:B:167:GLN:HB3	2:B:183:SER:HA	1.44	1.00
2:B:7:SER:HB3	2:B:8:PRO:CD	1.95	0.96
2:B:7:SER:HB3	2:B:8:PRO:HD3	1.48	0.96
3:C:163:SER:H	3:C:203:ASN:HD21	1.10	0.92
3:C:124:PRO:HB3	3:C:152:TYR:HB3	1.48	0.92
2:B:156:VAL:HG13	2:B:198:TYR:CE2	2.04	0.91
1:A:141:PRO:HA	1:A:144:ARG:HH11	1.32	0.91
2:B:158:GLY:C	2:B:159:SER:HG	1.77	0.88
2:B:181:LEU:HD23	2:B:182:SER:N	1.90	0.86
1:A:57:GLU:OE1	3:C:33:HIS:HE1	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:ARG:HG2	2:B:217:ARG:HH11	1.42	0.85
2:B:7:SER:CB	2:B:8:PRO:HD3	2.07	0.84
2:B:126:PRO:HB3	2:B:136:ALA:HB1	1.59	0.82
2:B:137:THR:HG22	2:B:186:SER:HA	1.62	0.80
1:A:329:SER:O	1:A:333:GLN:HB2	1.82	0.79
2:B:167:GLN:HB3	2:B:183:SER:CA	2.13	0.79
2:B:118:LYS:HG2	2:B:206:THR:CG2	2.13	0.79
2:B:155:LYS:NZ	2:B:158:GLY:O	2.15	0.78
3:C:53:ASN:N	3:C:53:ASN:HD22	1.82	0.78
1:A:129:PRO:HD2	1:A:181:ARG:O	1.84	0.78
3:C:33:HIS:HD2	3:C:53:ASN:H	1.29	0.77
2:B:137:THR:CG2	2:B:186:SER:HA	2.14	0.77
3:C:145:LEU:HD22	3:C:200:VAL:HG11	1.65	0.77
2:B:42:TYR:HE1	2:B:95:GLN:HG2	1.51	0.75
1:A:92:ARG:HB2	1:A:92:ARG:NH1	2.02	0.74
3:C:63:LEU:HD12	3:C:63:LEU:O	1.87	0.74
3:C:85:VAL:HG12	3:C:116:VAL:HG11	1.69	0.74
1:A:209:PHE:HB2	1:A:272:TRP:HB2	1.70	0.74
1:A:201:GLN:HB2	1:A:282:ILE:HD13	1.70	0.74
1:A:259:GLN:NE2	1:A:265:VAL:HG23	2.03	0.73
3:C:214:ASP:O	3:C:215:LYS:HG2	1.89	0.72
2:B:7:SER:HB2	2:B:22:SER:H	1.53	0.72
3:C:163:SER:H	3:C:203:ASN:ND2	1.86	0.72
2:B:98:ILE:O	2:B:98:ILE:HD13	1.90	0.72
2:B:7:SER:HB2	2:B:22:SER:HB3	1.72	0.71
3:C:163:SER:N	3:C:203:ASN:HD21	1.87	0.71
2:B:126:PRO:CB	2:B:136:ALA:HB1	2.21	0.71
1:A:168:ARG:HD2	1:A:311:LYS:HG2	1.73	0.70
2:B:7:SER:CB	2:B:22:SER:H	2.04	0.70
3:C:128:PRO:HB3	3:C:217:ILE:CD1	2.22	0.70
1:A:202:GLY:HA3	1:A:281:THR:HG22	1.75	0.69
3:C:39:GLN:NE2	3:C:43:LYS:HD2	2.08	0.69
3:C:53:ASN:H	3:C:53:ASN:HD22	1.40	0.68
2:B:2:ILE:HD13	2:B:99:SER:HB3	1.75	0.68
1:A:206:TRP:HB2	1:A:257:ILE:HB	1.75	0.68
1:A:332:LEU:C	1:A:334:GLU:H	1.96	0.68
2:B:124:PHE:CD1	3:C:129:LEU:HB3	2.29	0.68
1:A:326:LEU:O	1:A:329:SER:HB3	1.93	0.67
1:A:114:MET:HG3	1:A:118:ILE:HD11	1.76	0.67
2:B:67:ARG:NH2	2:B:88:ASP:OD1	2.26	0.67
1:A:284:ILE:HD13	1:A:285:THR:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HA	5:A:339:GOL:O2	1.95	0.66
1:A:92:ARG:HB2	1:A:92:ARG:HH11	1.60	0.66
1:A:91:LYS:HB2	1:A:118:ILE:HD13	1.78	0.66
1:A:89:ARG:HB3	1:A:89:ARG:HH11	1.60	0.65
2:B:34:ILE:HD12	3:C:103:TYR:CE2	2.31	0.65
1:A:142:LYS:HA	1:A:142:LYS:HE2	1.79	0.65
1:A:80:SER:OG	1:A:149:ASP:HA	1.97	0.65
2:B:217:ARG:NH1	2:B:217:ARG:HG2	2.12	0.65
2:B:43:GLN:HB2	2:B:53:LEU:HD11	1.79	0.64
2:B:151:ASN:HD21	2:B:153:LYS:HE3	1.62	0.64
2:B:125:PRO:HB2	2:B:126:PRO:CD	2.28	0.63
2:B:150:ILE:HG13	2:B:151:ASN:N	2.14	0.63
1:A:135:SER:HB3	1:A:174:TRP:CD1	2.32	0.63
2:B:67:ARG:HH21	2:B:88:ASP:CG	2.01	0.63
2:B:39:LEU:HD22	2:B:77:TYR:CG	2.34	0.63
2:B:137:THR:HG22	2:B:187:LEU:H	1.63	0.62
1:A:280:THR:H	5:A:338:GOL:H11	1.63	0.62
2:B:156:VAL:HG11	2:B:195:HIS:CG	2.35	0.62
3:C:90:THR:HG23	3:C:115:THR:HA	1.82	0.62
2:B:118:LYS:HG2	2:B:206:THR:HG21	1.81	0.61
3:C:99:ASP:HB3	3:C:102:THR:HG21	1.81	0.61
3:C:191:PRO:HG2	3:C:194:THR:HG22	1.82	0.61
3:C:170:VAL:O	3:C:171:HIS:HD2	1.82	0.61
2:B:39:LEU:HD22	2:B:77:TYR:CD1	2.35	0.61
3:C:157:VAL:HG23	3:C:184:LEU:HD21	1.82	0.61
3:C:190:VAL:HB	3:C:191:PRO:HD2	1.81	0.61
1:A:141:PRO:HA	1:A:144:ARG:NH1	2.09	0.61
2:B:126:PRO:HB2	2:B:131:LEU:HD11	1.83	0.60
1:A:129:PRO:CD	1:A:181:ARG:O	2.48	0.60
2:B:7:SER:HB2	2:B:22:SER:N	2.16	0.60
3:C:128:PRO:HG3	3:C:215:LYS:HB3	1.84	0.60
2:B:6:GLN:HE21	2:B:105:GLY:HA3	1.67	0.60
2:B:118:LYS:HA	2:B:206:THR:HG21	1.83	0.59
2:B:198:TYR:O	2:B:214:THR:HG23	2.01	0.59
1:A:301:THR:HG22	1:A:309:SER:HB3	1.85	0.59
2:B:124:PHE:HD1	3:C:129:LEU:HB3	1.66	0.59
2:B:121:VAL:HG12	2:B:122:SER:O	2.03	0.58
3:C:180:GLY:O	3:C:181:LEU:HD23	2.02	0.58
1:A:62:ARG:HH11	1:A:62:ARG:HG3	1.69	0.57
2:B:96:GLN:HE21	2:B:103:THR:H	1.52	0.57
1:A:133:PHE:CD1	1:A:133:PHE:O	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLN:CB	1:A:282:ILE:HD13	2.35	0.57
3:C:33:HIS:CD2	3:C:53:ASN:H	2.17	0.57
2:B:193:GLU:HA	2:B:217:ARG:HE	1.70	0.56
3:C:142:THR:HA	3:C:192:SER:HB2	1.88	0.56
3:C:128:PRO:HB3	3:C:217:ILE:HD13	1.88	0.56
1:A:112:MET:CE	1:A:117:TYR:HA	2.36	0.56
1:A:186:ILE:HD13	1:A:218:ILE:HD12	1.86	0.56
1:A:332:LEU:O	1:A:334:GLU:N	2.39	0.56
3:C:51:ILE:HD11	3:C:71:ARG:HD2	1.88	0.56
1:A:282:ILE:HD12	1:A:282:ILE:N	2.20	0.56
2:B:110:LEU:HD23	2:B:110:LEU:C	2.27	0.55
2:B:123:ILE:HG12	2:B:213:LYS:HB3	1.89	0.55
2:B:7:SER:HB2	2:B:22:SER:CB	2.37	0.55
2:B:7:SER:HB2	2:B:22:SER:CA	2.37	0.55
1:A:57:GLU:OE1	3:C:33:HIS:CE1	2.50	0.55
1:A:140:HIS:HD2	1:A:142:LYS:H	1.54	0.54
1:A:266:PHE:CE2	1:A:268:PRO:HG3	2.42	0.54
3:C:38:ARG:HB3	3:C:48:MET:HE1	1.88	0.54
1:A:1:MET:HG2	1:A:6:LYS:HD2	1.90	0.54
1:A:332:LEU:C	1:A:334:GLU:N	2.61	0.54
2:B:121:VAL:HG12	2:B:122:SER:N	2.22	0.54
2:B:34:ILE:HD12	3:C:103:TYR:HE2	1.73	0.53
1:A:10:ARG:HH11	1:A:14:ARG:HH21	1.57	0.53
2:B:156:VAL:CG1	2:B:198:TYR:CE2	2.86	0.53
1:A:284:ILE:HD13	1:A:285:THR:H	1.71	0.53
2:B:123:ILE:CG1	2:B:213:LYS:HB3	2.40	0.52
1:A:131:TYR:OH	1:A:184:THR:HG22	2.09	0.52
3:C:53:ASN:N	3:C:53:ASN:ND2	2.54	0.52
2:B:202:VAL:O	2:B:211:ILE:HG23	2.09	0.52
2:B:121:VAL:HA	2:B:141:PHE:O	2.10	0.52
1:A:48:ARG:HG2	1:A:71:VAL:HB	1.92	0.51
2:B:120:THR:HG23	2:B:120:THR:O	2.11	0.51
1:A:199:LEU:HD13	1:A:204:LYS:HE2	1.92	0.50
3:C:177:LEU:HD23	3:C:177:LEU:H	1.75	0.50
1:A:115:LYS:O	1:A:119:GLU:HG3	2.11	0.50
2:B:193:GLU:CB	2:B:217:ARG:HH21	2.25	0.50
3:C:166:LEU:HD13	3:C:188:VAL:HG21	1.92	0.50
1:A:2:ASN:OD1	1:A:4:LYS:HB2	2.12	0.50
2:B:199:THR:HG22	2:B:214:THR:OG1	2.11	0.50
3:C:177:LEU:HA	3:C:181:LEU:O	2.12	0.50
1:A:209:PHE:CE1	1:A:254:PRO:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:GLN:HE22	2:B:93:PHE:HA	1.77	0.50
2:B:167:GLN:HE21	2:B:181:LEU:HD11	1.76	0.50
3:C:157:VAL:CG2	3:C:184:LEU:HD21	2.41	0.50
1:A:6:LYS:HA	5:A:339:GOL:O1	2.11	0.49
2:B:11:LEU:HD12	2:B:11:LEU:C	2.32	0.49
1:A:180:PRO:O	1:A:181:ARG:HB2	2.12	0.49
1:A:108:TYR:CD2	1:A:108:TYR:N	2.79	0.49
2:B:8:PRO:O	2:B:108:THR:HG23	2.12	0.49
1:A:212:SER:HB2	1:A:252:PHE:HE1	1.78	0.49
2:B:7:SER:CB	2:B:22:SER:HB3	2.40	0.49
2:B:42:TYR:CE1	2:B:95:GLN:HG2	2.40	0.49
1:A:208:LEU:CD2	1:A:273:HIS:HB3	2.43	0.49
2:B:193:GLU:HA	2:B:217:ARG:HH21	1.77	0.49
2:B:150:ILE:CD1	2:B:204:HIS:HB2	2.43	0.49
3:C:191:PRO:HG2	3:C:194:THR:CG2	2.43	0.49
2:B:8:PRO:HG3	2:B:11:LEU:HD23	1.95	0.48
1:A:112:MET:HE2	1:A:117:TYR:N	2.28	0.48
3:C:161:TRP:HB3	3:C:166:LEU:HD12	1.94	0.48
3:C:126:VAL:HG21	3:C:213:VAL:HG21	1.95	0.48
2:B:133:THR:C	2:B:135:SER:H	2.17	0.48
2:B:100:ASN:OD1	3:C:61:PRO:HD3	2.12	0.48
2:B:162:ARG:O	2:B:162:ARG:HG2	2.13	0.48
1:A:201:GLN:HB2	1:A:282:ILE:CD1	2.41	0.48
2:B:86:ALA:HA	2:B:112:ILE:HD13	1.95	0.48
2:B:217:ARG:NH1	2:B:217:ARG:CG	2.77	0.48
1:A:112:MET:HE2	1:A:117:TYR:CA	2.43	0.48
3:C:3:GLN:HB2	3:C:25:THR:OG1	2.14	0.48
1:A:93:LYS:HD2	6:A:353:SO4:O1	2.13	0.47
2:B:196:ASN:O	2:B:217:ARG:CB	2.62	0.47
3:C:50:TYR:HE1	3:C:105:PHE:HE1	1.61	0.47
3:C:145:LEU:HD12	3:C:145:LEU:N	2.29	0.47
3:C:195:TRP:C	3:C:195:TRP:CD1	2.84	0.47
2:B:84:VAL:HG12	2:B:85:GLN:N	2.29	0.47
1:A:113:LYS:HD2	1:A:115:LYS:HE2	1.95	0.47
2:B:139:VAL:HG12	2:B:140:CYS:N	2.30	0.47
1:A:257:ILE:N	1:A:257:ILE:HD12	2.28	0.47
2:B:121:VAL:HG12	2:B:122:SER:H	1.78	0.47
1:A:300:LYS:HE3	6:A:348:SO4:O4	2.15	0.47
1:A:302:VAL:HG23	1:A:303:ARG:N	2.29	0.47
2:B:128:SER:HA	2:B:131:LEU:HD22	1.96	0.47
2:B:124:PHE:HZ	3:C:144:THR:O	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:HIS:HD2	3:C:53:ASN:N	2.04	0.47
1:A:70:VAL:HG22	1:A:71:VAL:N	2.30	0.47
2:B:13:VAL:HG11	2:B:19:VAL:HB	1.96	0.47
1:A:188:ILE:HD11	1:A:272:TRP:CE2	2.50	0.46
3:C:195:TRP:HB3	3:C:196:PRO:CD	2.44	0.46
3:C:128:PRO:CG	3:C:215:LYS:HD2	2.43	0.46
3:C:35:SER:HB2	3:C:50:TYR:CD1	2.50	0.46
2:B:7:SER:OG	2:B:8:PRO:HD3	2.14	0.46
1:A:199:LEU:HD21	1:A:202:GLY:O	2.16	0.46
2:B:123:ILE:HG12	2:B:213:LYS:CB	2.45	0.46
3:C:159:VAL:HA	3:C:203:ASN:O	2.15	0.46
3:C:126:VAL:HG21	3:C:213:VAL:CG2	2.46	0.46
1:A:91:LYS:O	1:A:95:ARG:HB2	2.15	0.46
1:A:186:ILE:CD1	1:A:218:ILE:HD12	2.46	0.46
2:B:133:THR:HG22	2:B:134:GLY:H	1.79	0.46
3:C:14:PRO:O	3:C:15:SER:HB2	2.16	0.46
3:C:62:SER:OG	3:C:63:LEU:N	2.48	0.46
3:C:85:VAL:HG12	3:C:116:VAL:CG1	2.44	0.46
1:A:281:THR:C	1:A:282:ILE:HD12	2.36	0.46
2:B:188:THR:HG22	2:B:190:ALA:H	1.81	0.46
1:A:18:PRO:HG2	1:A:105:ASN:ND2	2.31	0.46
3:C:152:TYR:CE2	3:C:157:VAL:HG13	2.51	0.46
3:C:162:ASN:HB2	3:C:165:ALA:HB3	1.97	0.46
2:B:128:SER:O	2:B:131:LEU:HB2	2.15	0.46
1:A:115:LYS:HE3	1:A:116:TYR:CE1	2.51	0.45
1:A:65:ARG:HG2	1:A:65:ARG:HH11	1.82	0.45
2:B:158:GLY:O	2:B:159:SER:CB	2.59	0.45
2:B:11:LEU:O	2:B:11:LEU:HD12	2.16	0.45
3:C:85:VAL:CG1	3:C:116:VAL:HG21	2.46	0.45
1:A:140:HIS:CD2	1:A:142:LYS:H	2.33	0.45
3:C:99:ASP:HB3	3:C:102:THR:CG2	2.46	0.45
3:C:18:LEU:HD12	3:C:19:THR:N	2.31	0.45
3:C:63:LEU:O	3:C:63:LEU:CD1	2.61	0.45
3:C:29:ILE:HD11	3:C:73:ILE:HA	1.98	0.45
2:B:156:VAL:HG13	2:B:198:TYR:HE2	1.70	0.45
3:C:184:LEU:HD12	3:C:184:LEU:C	2.37	0.45
2:B:118:LYS:HG2	2:B:206:THR:HG23	1.95	0.45
2:B:19:VAL:HG12	2:B:81:ILE:HB	1.99	0.45
2:B:55:TYR:CZ	2:B:59:THR:HG21	2.51	0.45
2:B:197:LEU:HD11	2:B:216:ASN:OD1	2.17	0.45
1:A:143:ARG:C	1:A:145:LYS:N	2.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:LYS:O	2:B:193:GLU:HG3	2.18	0.44
2:B:196:ASN:O	2:B:217:ARG:HB3	2.17	0.44
3:C:47:TRP:CZ2	3:C:49:GLY:HA2	2.52	0.44
1:A:169:ARG:HA	1:A:170:PRO:HD3	1.89	0.44
2:B:6:GLN:NE2	2:B:107:GLY:H	2.15	0.44
2:B:128:SER:HA	2:B:131:LEU:HB2	1.99	0.44
2:B:181:LEU:HD23	2:B:182:SER:H	1.79	0.44
1:A:305:ARG:O	1:A:308:LEU:HB3	2.18	0.44
1:A:81:ALA:HB1	1:A:85:TRP:CD2	2.53	0.44
3:C:154:PRO:O	3:C:206:HIS:HE1	2.01	0.44
1:A:46:VAL:HG21	1:A:257:ILE:HG13	1.98	0.44
1:A:208:LEU:HD23	1:A:273:HIS:CB	2.47	0.44
1:A:35:PHE:CD2	1:A:233:ILE:HD11	2.52	0.44
1:A:100:LYS:HE2	1:A:133:PHE:CE1	2.52	0.44
2:B:123:ILE:CG1	2:B:213:LYS:CB	2.96	0.43
2:B:86:ALA:HA	2:B:112:ILE:CD1	2.48	0.43
2:B:165:VAL:HA	2:B:184:THR:O	2.18	0.43
2:B:126:PRO:HB2	2:B:131:LEU:CD1	2.47	0.43
3:C:61:PRO:O	3:C:62:SER:O	2.36	0.43
1:A:114:MET:HG3	1:A:118:ILE:CD1	2.46	0.43
2:B:12:ALA:HA	2:B:111:GLU:O	2.19	0.43
2:B:125:PRO:HA	2:B:138:LEU:CD2	2.27	0.43
1:A:291:SER:HB2	2:B:32:SER:OG	2.18	0.43
2:B:137:THR:HG22	2:B:186:SER:CA	2.43	0.43
3:C:6:GLU:HA	3:C:21:THR:O	2.19	0.43
1:A:140:HIS:HA	1:A:141:PRO:HD2	1.80	0.43
1:A:8:ARG:HD3	1:A:8:ARG:HA	1.79	0.43
2:B:133:THR:HG22	2:B:134:GLY:N	2.33	0.43
2:B:197:LEU:HD12	2:B:197:LEU:N	2.34	0.43
2:B:123:ILE:C	2:B:124:PHE:CD2	2.92	0.43
1:A:132:ILE:HD12	1:A:177:MET:HB3	1.99	0.43
1:A:196:TRP:HA	1:A:265:VAL:O	2.19	0.42
1:A:286:GLN:HB3	1:A:286:GLN:HE21	1.52	0.42
2:B:60:LEU:HD21	2:B:64:VAL:O	2.19	0.42
2:B:196:ASN:ND2	2:B:197:LEU:CD1	2.82	0.42
1:A:7:LYS:HG3	1:A:10:ARG:NH2	2.34	0.42
1:A:294:PHE:HB3	1:A:295:PRO:HD3	2.00	0.42
3:C:51:ILE:C	3:C:51:ILE:HD13	2.40	0.42
2:B:120:THR:HG22	2:B:143:ASN:O	2.19	0.42
2:B:137:THR:HG22	2:B:187:LEU:N	2.32	0.42
2:B:202:VAL:HG13	2:B:211:ILE:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:GLN:HB3	2:B:183:SER:CB	2.49	0.42
1:A:208:LEU:HD23	1:A:273:HIS:HB3	2.01	0.42
2:B:6:GLN:HE21	2:B:105:GLY:CA	2.33	0.42
1:A:108:TYR:HD2	1:A:108:TYR:N	2.17	0.42
3:C:85:VAL:HG12	3:C:86:THR:N	2.35	0.42
3:C:170:VAL:O	3:C:171:HIS:CD2	2.69	0.42
3:C:161:TRP:CB	3:C:166:LEU:HD12	2.50	0.42
2:B:134:GLY:O	2:B:188:THR:HG23	2.20	0.42
1:A:55:SER:HB3	3:C:100:TYR:HE1	1.84	0.42
3:C:66:ARG:O	3:C:82:LEU:HA	2.20	0.42
3:C:2:ILE:HD13	3:C:27:ASP:HB2	2.02	0.41
2:B:199:THR:HG22	2:B:214:THR:CG2	2.51	0.41
1:A:89:ARG:CB	1:A:89:ARG:HH11	2.30	0.41
1:A:205:ARG:CZ	1:A:236:PHE:CE1	3.03	0.41
2:B:131:LEU:HD12	2:B:136:ALA:HB2	2.02	0.41
2:B:176:ASP:O	2:B:178:THR:HG23	2.21	0.41
2:B:25:SER:HB3	2:B:27:GLN:O	2.20	0.41
2:B:193:GLU:HG2	2:B:217:ARG:HH21	1.84	0.41
2:B:196:ASN:O	2:B:217:ARG:HB2	2.20	0.41
3:C:154:PRO:HD2	3:C:208:ALA:HB1	2.02	0.41
3:C:128:PRO:HG2	3:C:215:LYS:HD2	2.02	0.41
1:A:206:TRP:CD2	1:A:275:VAL:HG22	2.56	0.41
2:B:130:GLN:HB2	3:C:127:TYR:CG	2.55	0.41
3:C:53:ASN:H	3:C:53:ASN:ND2	2.12	0.41
2:B:123:ILE:O	2:B:124:PHE:HD2	2.03	0.41
1:A:5:SER:O	1:A:6:LYS:C	2.59	0.41
1:A:300:LYS:HE3	6:A:348:SO4:S	2.61	0.41
2:B:54:ILE:HD12	2:B:79:LEU:CD1	2.50	0.41
3:C:206:HIS:HD2	3:C:209:SER:OG	2.03	0.41
1:A:321:PRO:O	1:A:325:VAL:HG23	2.21	0.41
2:B:167:GLN:NE2	2:B:181:LEU:HD11	2.36	0.41
1:A:120:TYR:O	1:A:124:THR:HG22	2.20	0.41
3:C:51:ILE:HG23	3:C:51:ILE:O	2.21	0.41
1:A:2:ASN:O	1:A:4:LYS:N	2.54	0.41
1:A:248:TRP:HA	1:A:249:PRO:HD3	1.92	0.40
2:B:165:VAL:HB	2:B:185:LEU:HD13	2.03	0.40
1:A:26:TRP:HB3	1:A:126:ASP:OD1	2.20	0.40
1:A:280:THR:N	5:A:338:GOL:H11	2.34	0.40
3:C:142:THR:HG23	3:C:142:THR:O	2.22	0.40
2:B:188:THR:HB	2:B:191:ASP:OD2	2.22	0.40
1:A:255:LEU:HD12	1:A:255:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:GLU:CA	2:B:217:ARG:HH21	2.35	0.40
1:A:330:VAL:HA	1:A:333:GLN:HB3	2.04	0.40
2:B:52:LEU:HD13	2:B:61:PHE:CG	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	307 (92%)	19 (6%)	6 (2%)	11	27
2	B	215/220 (98%)	183 (85%)	23 (11%)	9 (4%)	3	7
3	C	206/221 (93%)	170 (82%)	27 (13%)	9 (4%)	3	6
All	All	753/775 (97%)	660 (88%)	69 (9%)	24 (3%)	5	12

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	7	SER
2	B	163	ASP
2	B	206	THR
3	C	62	SER
3	C	119	ALA
3	C	167	THR
3	C	194	THR
1	A	3	HIS
1	A	124	THR
1	A	333	GLN
2	B	211	ILE
3	C	43	LYS
3	C	193	SER
3	C	195	TRP

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Mol	Chain	Res	Type
2	B	123	ILE
2	B	125	PRO
1	A	159	ASP
3	C	166	LEU
1	A	216	GLU
2	B	8	PRO
1	A	306	PRO
2	B	156	VAL
2	B	74	GLY
3	C	156	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/301 (100%)	288 (96%)	13 (4%)	35	66
2	B	190/193 (98%)	179 (94%)	11 (6%)	25	52
3	C	187/196 (95%)	178 (95%)	9 (5%)	31	62
All	All	678/690 (98%)	645 (95%)	33 (5%)	31	61

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	57	GLU
1	A	62	ARG
1	A	89	ARG
1	A	92	ARG
1	A	158	ASP
1	A	161	PHE
1	A	207	CYS
1	A	212	SER
1	A	255	LEU
1	A	284	ILE
1	A	285	THR

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Mol	Chain	Res	Type
1	A	326	LEU
2	B	1	ASP
2	B	34	ILE
2	B	39	LEU
2	B	44	LEU
2	B	52	LEU
2	B	83	SER
2	B	95	GLN
2	B	98	ILE
2	B	156	VAL
2	B	167	GLN
2	B	215	LEU
3	C	51	ILE
3	C	53	ASN
3	C	66	ARG
3	C	71	ARG
3	C	147	CYS
3	C	156	PRO
3	C	159	VAL
3	C	176	VAL
3	C	202	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	277	ASN
1	A	286	GLN
2	B	6	GLN
2	B	85	GLN
2	B	143	ASN
2	B	151	ASN
2	B	167	GLN
2	B	196	ASN
3	C	33	HIS
3	C	39	GLN
3	C	53	ASN
3	C	81	GLN
3	C	141	ASN
3	C	171	HIS
3	C	203	ASN
3	C	206	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 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	$\# Z  > 2$
5	GOL	A	337	-	5,5,5	0.41	0	5,5,5	0.26	0
5	GOL	A	338	-	5,5,5	0.22	0	5,5,5	0.27	0
5	GOL	A	339	-	5,5,5	0.30	0	5,5,5	0.29	0
5	GOL	A	340	-	5,5,5	0.28	0	5,5,5	0.26	0
6	SO4	A	341	-	4,4,4	0.24	0	6,6,6	0.16	0
6	SO4	A	342	-	4,4,4	0.23	0	6,6,6	0.14	0
6	SO4	A	343	-	4,4,4	0.19	0	6,6,6	0.11	0
6	SO4	A	344	-	4,4,4	0.18	0	6,6,6	0.07	0
6	SO4	A	345	-	4,4,4	0.18	0	6,6,6	0.07	0
6	SO4	A	346	-	4,4,4	0.23	0	6,6,6	0.15	0
6	SO4	A	347	-	4,4,4	0.21	0	6,6,6	0.08	0
6	SO4	A	348	-	4,4,4	0.22	0	6,6,6	0.11	0
6	SO4	A	349	-	4,4,4	0.22	0	6,6,6	0.07	0
6	SO4	A	350	-	4,4,4	0.20	0	6,6,6	0.07	0
6	SO4	A	351	-	4,4,4	0.18	0	6,6,6	0.27	0
6	SO4	A	352	-	4,4,4	0.20	0	6,6,6	0.10	0
6	SO4	A	353	-	4,4,4	0.19	0	6,6,6	0.07	0
6	SO4	A	354	-	4,4,4	0.21	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	B	221	-	5,5,5	0.30	0	5,5,5	0.26	0
6	SO4	B	222	-	4,4,4	0.21	0	6,6,6	0.10	0
6	SO4	B	223	-	4,4,4	0.19	0	6,6,6	0.10	0
6	SO4	C	222	-	4,4,4	0.26	0	6,6,6	0.13	0
6	SO4	C	223	-	4,4,4	0.18	0	6,6,6	0.09	0
6	SO4	C	224	-	4,4,4	0.19	0	6,6,6	0.08	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
5	GOL	A	337	-	-	0/4/4/4	0/0/0/0
5	GOL	A	338	-	-	0/4/4/4	0/0/0/0
5	GOL	A	339	-	-	0/4/4/4	0/0/0/0
5	GOL	A	340	-	-	0/4/4/4	0/0/0/0
6	SO4	A	341	-	-	0/0/0/0	0/0/0/0
6	SO4	A	342	-	-	0/0/0/0	0/0/0/0
6	SO4	A	343	-	-	0/0/0/0	0/0/0/0
6	SO4	A	344	-	-	0/0/0/0	0/0/0/0
6	SO4	A	345	-	-	0/0/0/0	0/0/0/0
6	SO4	A	346	-	-	0/0/0/0	0/0/0/0
6	SO4	A	347	-	-	0/0/0/0	0/0/0/0
6	SO4	A	348	-	-	0/0/0/0	0/0/0/0
6	SO4	A	349	-	-	0/0/0/0	0/0/0/0
6	SO4	A	350	-	-	0/0/0/0	0/0/0/0
6	SO4	A	351	-	-	0/0/0/0	0/0/0/0
6	SO4	A	352	-	-	0/0/0/0	0/0/0/0
6	SO4	A	353	-	-	0/0/0/0	0/0/0/0
6	SO4	A	354	-	-	0/0/0/0	0/0/0/0
5	GOL	B	221	-	-	0/4/4/4	0/0/0/0
6	SO4	B	222	-	-	0/0/0/0	0/0/0/0
6	SO4	B	223	-	-	0/0/0/0	0/0/0/0
6	SO4	C	222	-	-	0/0/0/0	0/0/0/0
6	SO4	C	223	-	-	0/0/0/0	0/0/0/0
6	SO4	C	224	-	-	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.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	338	GOL	2	0
5	A	339	GOL	2	0
6	A	348	SO4	2	0
6	A	353	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/334 (100%)	0.23	5 (1%)	76	76	41, 66, 105, 130	4 (1%)
2	B	217/220 (98%)	0.68	21 (9%)	10	7	36, 74, 144, 151	0
3	C	210/221 (95%)	0.63	25 (11%)	6	5	35, 83, 131, 140	0
All	All	761/775 (98%)	0.47	51 (6%)	21	19	35, 71, 135, 151	4 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	145	LEU	8.2
2	B	123	ILE	6.9
2	B	163	ASP	5.9
2	B	201	GLU	5.3
2	B	209	ALA	5.0
3	C	199	THR	4.9
2	B	215	LEU	4.5
1	A	1	MET	4.5
3	C	217	ILE	4.1
2	B	155	LYS	4.0
2	B	122	SER	3.8
3	C	216	LYS	3.7
2	B	211	ILE	3.6
3	C	218	VAL	3.5
3	C	197	SER	3.3
1	A	133	PHE	3.3
2	B	162	ARG	3.3
3	C	143	VAL	3.2
3	C	162	ASN	3.2
2	B	210	ALA	3.2
3	C	190	VAL	3.2
3	C	166	LEU	3.1
2	B	198	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	198	GLN	3.1
3	C	128	PRO	3.0
2	B	156	VAL	3.0
2	B	203	THR	3.0
3	C	164	GLY	3.0
1	A	333	GLN	3.0
3	C	151	GLY	3.0
1	A	334	GLU	2.9
2	B	157	ASP	2.8
2	B	202	VAL	2.8
3	C	196	PRO	2.6
2	B	121	VAL	2.6
3	C	192	SER	2.6
2	B	185	LEU	2.6
2	B	124	PHE	2.5
2	B	154	TRP	2.5
3	C	127	TYR	2.4
3	C	194	THR	2.4
3	C	18	LEU	2.3
3	C	195	TRP	2.3
1	A	314	ARG	2.3
3	C	131	PRO	2.2
3	C	219	PRO	2.2
3	C	146	GLY	2.2
2	B	153	LYS	2.1
3	C	165	ALA	2.1
2	B	189	LYS	2.0
3	C	188	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	337	6/6	0.65	0.40	11.35	104,106,109,111	0
6	SO4	A	341	5/5	0.87	0.40	7.26	59,60,63,63	5
6	SO4	B	223	5/5	0.89	0.28	4.52	111,111,111,112	5
6	SO4	C	223	5/5	0.92	0.32	3.34	57,57,58,58	5
5	GOL	A	339	6/6	0.82	0.41	1.62	93,95,97,97	0
6	SO4	A	343	5/5	0.84	0.17	-0.46	132,132,133,133	0
4	HG	A	335	1/1	0.97	0.15	-1.38	92,92,92,92	1
6	SO4	A	349	5/5	0.89	0.25	-	157,157,157,157	0
6	SO4	C	224	5/5	0.77	0.31	-	183,183,183,183	0
6	SO4	A	352	5/5	0.85	0.19	-	103,103,103,104	5
6	SO4	A	345	5/5	0.82	0.17	-	157,157,158,158	0
6	SO4	B	222	5/5	0.92	0.24	-	74,74,75,75	5
5	GOL	A	340	6/6	0.81	0.30	-	113,115,115,115	0
6	SO4	A	347	5/5	0.73	0.20	-	168,168,169,169	0
6	SO4	A	351	5/5	0.95	0.16	-	91,92,94,96	0
5	GOL	A	338	6/6	0.92	0.14	-	77,79,81,83	0
6	SO4	A	342	5/5	0.90	0.17	-	139,140,140,140	0
6	SO4	A	346	5/5	0.93	0.13	-	139,140,140,141	0
5	GOL	B	221	6/6	0.74	0.17	-	116,118,119,119	0
6	SO4	A	344	5/5	0.90	0.22	-	146,146,146,147	0
6	SO4	A	350	5/5	0.96	0.19	-	153,153,154,154	0
6	SO4	A	348	5/5	0.91	0.20	-	76,77,77,78	5
4	HG	A	336	1/1	0.95	0.13	-	115,115,115,115	1
7	FE	A	601	1/1	0.80	0.27	-	148,148,148,148	0
6	SO4	A	354	5/5	0.85	0.29	-	175,175,175,175	0
6	SO4	C	222	5/5	0.85	0.23	-	74,75,76,76	5
6	SO4	A	353	5/5	0.92	0.10	-	131,132,132,132	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.