



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:39 AM GMT

PDB ID : 3E4B  
Title : Crystal structure of AlgK from Pseudomonas fluorescens WCS374r  
Authors : Keiski, C.-L.; Harwich, M.; Jain, S.; Neculai, A.M.; Yip, P.; Robinson, H.; Whitney, J.C.; Burrows, L.L.; Ohman, D.E.; Howell, P.L.  
Deposited on : 2008-08-11  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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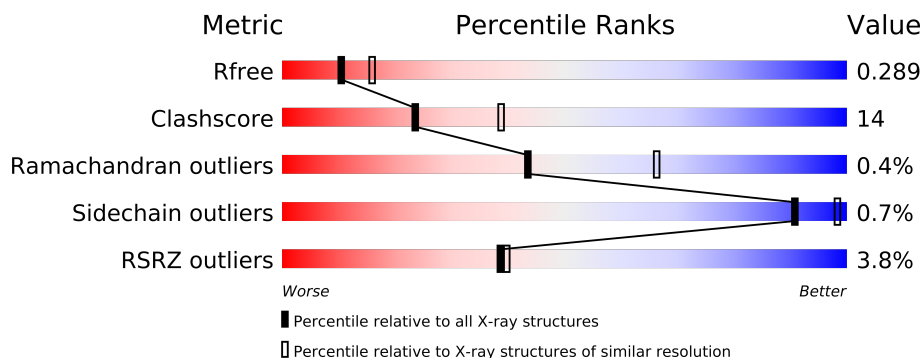
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	452	
1	B	452	
1	C	452	
1	D	452	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	B	453	-	X
3	GOL	C	455	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12341 atoms, of which 0 are hydrogen and 0 are deuterium.

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 AlgK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			2988	1877	526	579	6			
1	B	405	Total	C	N	O	S	0	0	0
			3045	1915	530	594	6			
1	C	405	Total	C	N	O	S	0	0	0
			3057	1918	533	600	6			
1	D	316	Total	C	N	O	S	0	0	0
			2371	1493	407	466	5			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 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
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

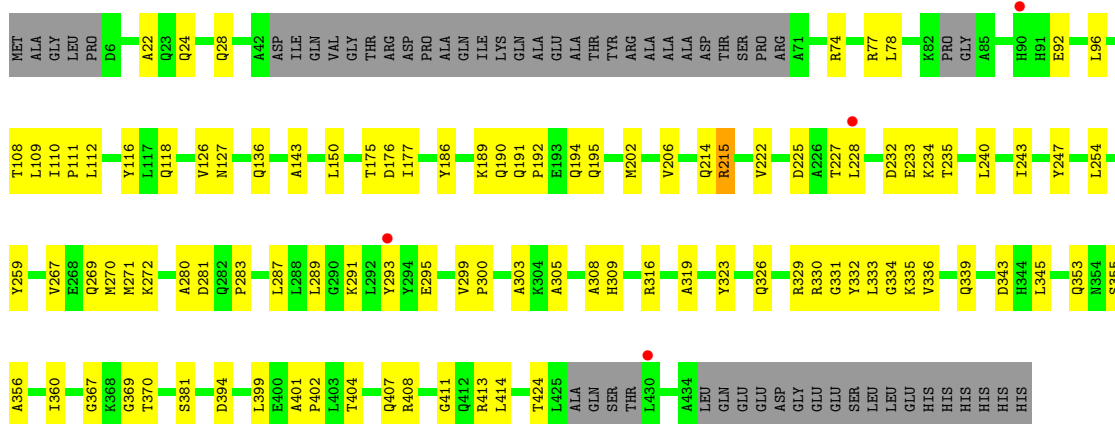
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	197	Total	O	0	0
			197	197		
4	B	222	Total	O	0	0
			222	222		
4	C	302	Total	O	0	0
			302	302		
4	D	132	Total	O	0	0
			132	132		

### 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.

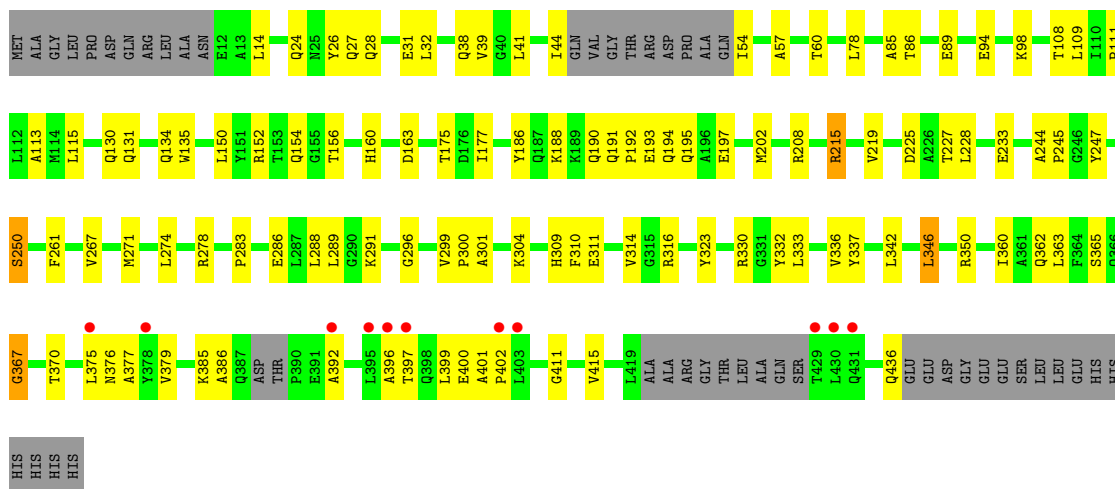
#### • Molecule 1: AlgK

Chain A: 



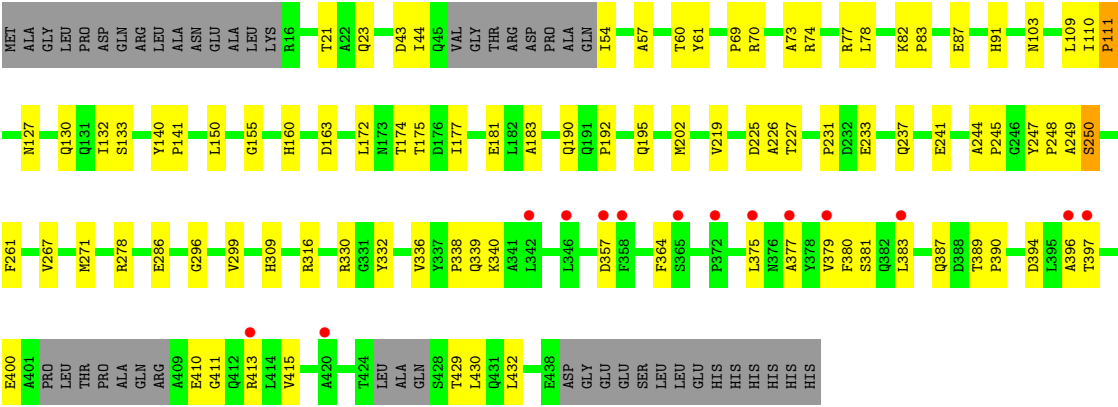
#### • Molecule 1: AlgK

Chain B: 



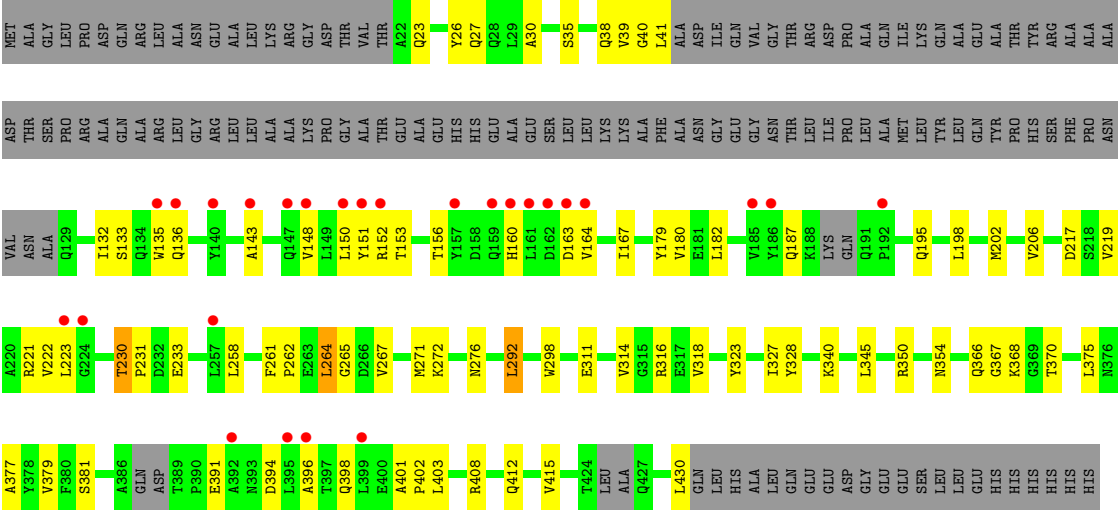
#### • Molecule 1: AlgK

Chain C: 



● Molecule 1: AlgK

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.09Å 107.82Å 119.03Å 90.00° 96.97° 90.00°	Depositor
Resolution (Å)	49.05 – 2.50 49.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.05-2.50) 100.0 (49.05-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.05 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.220 , 0.280 0.232 , 0.289	Depositor DCC
$R_{free}$ test set	3540 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 68663 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12341	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	A	0.46	0/3039	0.66	0/4129
1	B	0.50	0/3100	0.67	1/4217 (0.0%)
1	C	0.53	0/3111	0.68	0/4230
1	D	0.50	0/2411	0.70	2/3277 (0.1%)
All	All	0.50	0/11661	0.68	3/15853 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	292	LEU	CA-CB-CG	5.51	127.98	115.30
1	B	215	ARG	CG-CD-NE	-5.28	100.72	111.80
1	D	264	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2988	0	2888	83	0
1	B	3045	0	2896	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3057	0	2913	96	0
1	D	2371	0	2243	65	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	B	6	0	8	0	0
3	C	12	0	16	0	0
3	D	6	0	8	0	0
4	A	197	0	0	7	0
4	B	222	0	0	7	0
4	C	302	0	0	6	0
4	D	132	0	0	3	0
All	All	12341	0	10972	324	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (324) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:202:MET:HE3	1:B:219:VAL:HG21	1.30	1.09
1:B:202:MET:CE	1:B:219:VAL:HG21	2.02	0.90
1:C:387:GLN:HG2	1:C:389:THR:HG23	1.52	0.90
1:A:191:GLN:HB3	1:A:194:GLN:OE1	1.72	0.89
1:C:330:ARG:HB3	1:C:330:ARG:HH11	1.39	0.85
1:C:233:GLU:HG2	1:C:261:PHE:CD1	2.13	0.84
1:A:303:ALA:HB1	1:A:333:LEU:HD23	1.59	0.83
1:B:191:GLN:HB3	1:B:194:GLN:OE1	1.76	0.83
1:C:336:VAL:O	1:C:338:PRO:HD3	1.78	0.83
1:C:60:THR:HG23	1:C:61:TYR:H	1.43	0.83
1:B:60:THR:HB	4:B:716:HOH:O	1.77	0.83
1:C:202:MET:CE	1:C:219:VAL:HG21	2.10	0.82
1:B:274:LEU:O	1:B:278:ARG:HG3	1.78	0.82
1:D:391:GLU:H	1:D:391:GLU:CD	1.84	0.80
1:D:148:VAL:HG22	1:D:164:VAL:HG22	1.63	0.79
1:B:233:GLU:HG2	1:B:261:PHE:CD1	2.20	0.77
1:B:367:GLY:HA2	1:B:370:THR:O	1.83	0.77
1:C:74:ARG:NH1	1:C:74:ARG:HB2	2.00	0.77
1:C:54:ILE:HG12	1:C:54:ILE:O	1.84	0.76
1:C:430:LEU:HB3	1:C:432:LEU:HD11	1.66	0.76
1:C:202:MET:HE3	1:C:219:VAL:HG21	1.67	0.75
1:C:390:PRO:O	1:C:394:ASP:HB2	1.87	0.75
1:A:214:GLN:HG2	1:A:214:GLN:O	1.88	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:226:ALA:HA	1:C:231:PRO:HG3	1.71	0.73
1:D:233:GLU:HB2	1:D:264:LEU:CD2	2.19	0.72
1:B:175:THR:HG22	1:B:177:ILE:HG22	1.72	0.72
1:D:202:MET:HE2	1:D:219:VAL:HG21	1.71	0.72
1:B:57:ALA:O	1:B:60:THR:HG22	1.90	0.71
1:B:26:TYR:CE1	1:B:41:LEU:HD11	2.25	0.71
1:B:311:GLU:O	1:B:314:VAL:HG22	1.91	0.71
1:A:335:LYS:HG2	1:A:336:VAL:H	1.54	0.71
1:B:278:ARG:HH11	1:B:278:ARG:HB3	1.54	0.71
1:B:225:ASP:OD1	1:B:227:THR:HB	1.91	0.70
1:A:331:GLY:HA3	1:A:336:VAL:HG22	1.71	0.70
1:B:26:TYR:CZ	1:B:41:LEU:HD11	2.27	0.69
1:C:339:GLN:HG3	1:C:340:LYS:H	1.56	0.69
1:D:233:GLU:HB2	1:D:264:LEU:HD23	1.73	0.69
1:A:369:GLY:C	1:B:436:GLN:HG3	2.11	0.69
1:A:22:ALA:HA	1:A:118:GLN:HE21	1.58	0.69
1:D:272:LYS:HE2	1:D:276:ASN:HD21	1.59	0.68
1:B:385:LYS:HA	1:B:392:ALA:HB1	1.74	0.68
1:C:183:ALA:HA	1:C:195:GLN:HE22	1.58	0.67
1:B:44:ILE:CG2	1:B:78:LEU:HD13	2.24	0.67
1:C:432:LEU:HD12	1:C:432:LEU:N	2.10	0.67
1:B:186:TYR:HB3	1:B:195:GLN:HG2	1.74	0.67
1:B:109:LEU:HD21	1:B:135:TRP:CE3	2.29	0.67
1:A:353:GLN:HE21	1:A:355:SER:HB2	1.59	0.66
1:A:299:VAL:HB	1:A:300:PRO:HD2	1.78	0.66
1:A:330:ARG:HD2	1:A:332:TYR:CZ	2.30	0.66
1:B:286:GLU:OE1	1:B:309:HIS:HD2	1.80	0.65
1:A:411:GLY:HA2	1:A:414:LEU:HD12	1.77	0.65
1:B:233:GLU:HG2	1:B:261:PHE:CG	2.31	0.65
1:C:87:GLU:HG2	1:C:91:HIS:CE1	2.32	0.65
1:A:413:ARG:HH11	1:A:413:ARG:HG2	1.62	0.64
1:B:160:HIS:HD2	1:B:163:ASP:OD2	1.80	0.64
1:D:318:VAL:HG23	4:D:704:HOH:O	1.98	0.64
1:C:57:ALA:HA	1:C:60:THR:HG22	1.79	0.64
1:C:375:LEU:O	1:C:379:VAL:HG23	1.98	0.64
1:C:60:THR:HG23	1:C:61:TYR:N	2.12	0.64
1:D:264:LEU:HD12	1:D:264:LEU:O	1.98	0.63
1:A:92:GLU:O	1:A:96:LEU:HG	1.99	0.63
1:C:411:GLY:O	1:C:415:VAL:HG23	1.98	0.63
1:B:190:GLN:O	1:B:192:PRO:HD3	1.99	0.63
1:C:364:PHE:HB2	1:C:377:ALA:HB2	1.81	0.62
1:C:330:ARG:HB3	1:C:330:ARG:NH1	2.10	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:233:GLU:HG2	1:C:261:PHE:CG	2.34	0.62
1:A:240:LEU:HB2	1:A:254:LEU:HD21	1.80	0.62
1:D:156:THR:HB	1:D:160:HIS:HE1	1.64	0.62
1:C:202:MET:HE1	1:C:219:VAL:HG21	1.82	0.61
1:C:247:TYR:O	1:C:250:SER:HB2	1.99	0.61
1:D:40:GLY:O	1:D:41:LEU:CB	2.48	0.61
1:C:57:ALA:O	1:C:60:THR:HG22	2.00	0.61
1:A:225:ASP:OD1	1:A:227:THR:HB	2.01	0.61
1:C:339:GLN:CG	1:C:340:LYS:H	2.14	0.60
1:A:291:LYS:O	1:A:295:GLU:HG2	2.01	0.60
1:D:202:MET:CE	1:D:219:VAL:HG21	2.31	0.60
1:B:291:LYS:HE3	1:B:323:TYR:OH	2.02	0.60
1:C:225:ASP:OD1	1:C:227:THR:HB	2.02	0.60
1:B:108:THR:C	1:B:111:PRO:HD2	2.21	0.59
1:B:208:ARG:HG2	1:B:208:ARG:HH11	1.67	0.59
1:B:32:LEU:HD21	1:B:152:ARG:CZ	2.32	0.59
1:A:335:LYS:HG2	1:A:336:VAL:N	2.18	0.59
1:C:387:GLN:HG2	1:C:389:THR:CG2	2.27	0.58
1:B:283:PRO:HD2	4:B:598:HOH:O	2.04	0.58
1:C:127:ASN:HB3	1:C:130:GLN:HB2	1.86	0.58
1:B:188:LYS:NZ	4:B:652:HOH:O	2.36	0.57
1:B:278:ARG:NH1	1:B:278:ARG:HB3	2.19	0.57
1:A:269:GLN:O	1:A:272:LYS:N	2.35	0.57
1:D:156:THR:HB	1:D:160:HIS:CE1	2.39	0.57
1:C:190:GLN:O	1:C:192:PRO:HD3	2.05	0.57
1:A:28:GLN:HB3	4:A:524:HOH:O	2.04	0.57
1:A:291:LYS:HE3	1:A:323:TYR:OH	2.04	0.57
1:B:299:VAL:HG22	1:B:300:PRO:HD2	1.87	0.57
1:B:57:ALA:O	1:B:60:THR:CG2	2.52	0.57
1:B:289:LEU:HD23	1:B:309:HIS:CD2	2.40	0.57
1:D:202:MET:HE1	1:D:219:VAL:HG11	1.85	0.57
1:A:186:TYR:CB	1:A:195:GLN:HG2	2.35	0.56
1:A:186:TYR:HB3	1:A:195:GLN:HG2	1.87	0.56
1:D:187:GLN:NE2	1:D:230:THR:O	2.39	0.56
1:D:153:THR:HG22	4:D:763:HOH:O	2.06	0.56
1:C:233:GLU:HG2	1:C:261:PHE:CE1	2.40	0.56
1:A:394:ASP:HB3	4:A:585:HOH:O	2.06	0.56
1:B:330:ARG:CZ	1:B:332:TYR:OH	2.54	0.55
1:C:330:ARG:NH1	1:C:332:TYR:CE1	2.75	0.55
1:D:35:SER:HG	1:D:38:GLN:CD	2.10	0.55
1:A:136:GLN:HG3	1:A:143:ALA:HB1	1.89	0.55
1:D:202:MET:O	1:D:206:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:377:ALA:HB1	1:B:399:LEU:HD13	1.88	0.55
1:C:155:GLY:HA2	4:C:609:HOH:O	2.06	0.55
1:B:296:GLY:HA2	1:B:299:VAL:O	2.07	0.55
1:C:110:ILE:HB	1:C:111:PRO:HD3	1.88	0.54
1:A:289:LEU:HD22	1:A:309:HIS:ND1	2.22	0.54
1:C:57:ALA:CA	1:C:60:THR:HG22	2.37	0.54
1:B:39:VAL:HG23	1:B:41:LEU:HD13	1.88	0.54
1:A:269:GLN:OE1	1:A:269:GLN:HA	2.08	0.54
1:A:283:PRO:HG3	1:A:316:ARG:CZ	2.37	0.54
1:C:57:ALA:O	1:C:60:THR:CG2	2.55	0.54
1:C:74:ARG:HH11	1:C:74:ARG:HB2	1.71	0.54
1:B:14:LEU:HD12	1:B:14:LEU:H	1.73	0.54
1:B:131:GLN:O	1:B:134:GLN:HB3	2.08	0.54
1:A:281:ASP:O	1:A:283:PRO:HD3	2.07	0.54
1:C:174:THR:HG23	4:C:720:HOH:O	2.08	0.54
1:D:375:LEU:O	1:D:379:VAL:HG23	2.08	0.54
1:A:331:GLY:CA	1:A:336:VAL:HG22	2.36	0.53
1:B:154:GLN:O	1:B:156:THR:HG23	2.07	0.53
1:A:289:LEU:O	1:A:289:LEU:HD23	2.09	0.53
1:A:326:GLN:OE1	1:A:326:GLN:HA	2.07	0.53
1:D:182:LEU:HB3	1:D:198:LEU:HD22	1.91	0.53
1:A:289:LEU:C	1:A:289:LEU:HD23	2.29	0.53
1:C:73:ALA:HB1	1:C:77:ARG:HH12	1.74	0.53
1:B:375:LEU:O	1:B:379:VAL:HG23	2.09	0.53
1:D:316:ARG:HG3	1:D:316:ARG:HH11	1.73	0.53
1:A:280:ALA:O	1:A:281:ASP:HB3	2.07	0.53
1:B:360:ILE:O	1:B:363:LEU:HB3	2.09	0.53
1:A:408:ARG:HD3	4:A:560:HOH:O	2.09	0.52
1:B:247:TYR:O	1:B:250:SER:HB2	2.09	0.52
1:B:44:ILE:O	1:B:44:ILE:HG22	2.09	0.52
1:C:109:LEU:O	1:C:109:LEU:HD23	2.09	0.52
1:A:175:THR:HG22	1:A:177:ILE:HG22	1.90	0.52
1:A:190:GLN:O	1:A:192:PRO:HD3	2.09	0.52
1:C:286:GLU:OE1	1:C:309:HIS:HD2	1.92	0.52
1:D:163:ASP:O	1:D:167:ILE:HG13	2.09	0.52
1:C:74:ARG:HH11	1:C:74:ARG:CB	2.23	0.52
1:B:86:THR:OG1	1:B:89:GLU:HG3	2.10	0.52
1:A:24:GLN:O	1:A:28:GLN:HG3	2.10	0.51
1:A:243:ILE:HB	4:A:646:HOH:O	2.10	0.51
1:A:289:LEU:HD21	1:A:293:TYR:CE2	2.45	0.51
1:A:110:ILE:HB	1:A:111:PRO:HD3	1.91	0.51
1:A:77:ARG:NH2	4:A:599:HOH:O	2.43	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:94:GLU:O	1:B:98:LYS:HG3	2.09	0.51
1:D:233:GLU:HB2	1:D:264:LEU:HD21	1.91	0.51
1:A:202:MET:O	1:A:206:VAL:HG23	2.11	0.51
1:B:44:ILE:HG22	1:B:78:LEU:HD13	1.92	0.51
1:D:367:GLY:HA2	1:D:370:THR:O	2.11	0.51
1:A:259:TYR:HE2	1:A:295:GLU:OE2	1.94	0.51
1:C:109:LEU:C	1:C:109:LEU:HD23	2.31	0.51
1:B:310:PHE:CE2	1:B:323:TYR:HB3	2.45	0.50
1:A:78:LEU:HD23	1:A:78:LEU:C	2.31	0.50
1:B:301:ALA:O	1:C:133:SER:OG	2.22	0.50
1:D:202:MET:HE2	1:D:219:VAL:CG2	2.41	0.50
1:D:132:ILE:HA	1:D:135:TRP:CE3	2.47	0.50
1:A:413:ARG:NH1	1:A:413:ARG:HG2	2.27	0.50
1:C:316:ARG:HH11	1:C:316:ARG:HG3	1.77	0.50
1:C:330:ARG:NH1	1:C:332:TYR:HE1	2.10	0.49
1:C:78:LEU:C	1:C:78:LEU:HD23	2.33	0.49
1:B:401:ALA:HB3	1:B:402:PRO:HD3	1.95	0.49
1:C:396:ALA:O	1:C:400:GLU:HG3	2.13	0.49
1:B:208:ARG:NH1	1:B:208:ARG:HG2	2.26	0.49
1:C:430:LEU:HB3	1:C:432:LEU:CD1	2.40	0.49
1:A:150:LEU:HD23	1:A:150:LEU:C	2.33	0.49
1:C:430:LEU:CB	1:C:432:LEU:HD11	2.41	0.49
1:C:175:THR:HG22	1:C:177:ILE:HG22	1.95	0.49
1:C:60:THR:CG2	1:C:61:TYR:H	2.20	0.48
1:B:38:GLN:NE2	1:B:177:ILE:HB	2.27	0.48
1:D:272:LYS:HE2	1:D:276:ASN:ND2	2.26	0.48
1:B:197:GLU:HA	1:B:197:GLU:OE1	2.14	0.48
1:D:258:LEU:HD11	1:D:265:GLY:HA3	1.95	0.48
1:A:401:ALA:HB3	1:A:402:PRO:HD3	1.95	0.48
1:B:396:ALA:O	1:B:400:GLU:HB2	2.14	0.48
1:D:39:VAL:HG23	1:D:40:GLY:N	2.28	0.48
1:B:24:GLN:O	1:B:28:GLN:HG3	2.13	0.48
1:D:354:ASN:N	1:D:354:ASN:OD1	2.47	0.48
1:D:366:GLN:O	1:D:368:LYS:HG2	2.13	0.48
1:D:403:LEU:O	1:D:408:ARG:NH2	2.38	0.48
1:C:57:ALA:HA	1:C:60:THR:CG2	2.44	0.48
1:D:30:ALA:HB2	4:D:699:HOH:O	2.14	0.48
1:B:130:GLN:HG3	4:B:660:HOH:O	2.14	0.48
1:C:57:ALA:C	1:C:60:THR:HG22	2.35	0.47
1:B:283:PRO:HG3	1:B:316:ARG:CZ	2.44	0.47
1:A:190:GLN:C	1:A:192:PRO:HD3	2.35	0.47
1:D:292:LEU:HD22	1:D:298:TRP:HB2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:411:GLY:O	1:B:415:VAL:HG23	2.14	0.47
1:D:179:TYR:CD1	1:D:198:LEU:HD11	2.49	0.47
1:B:27:GLN:O	1:B:31:GLU:HG2	2.14	0.47
1:B:278:ARG:HD2	1:B:286:GLU:OE2	2.14	0.47
1:C:397:THR:O	1:C:400:GLU:HB2	2.15	0.47
1:B:436:GLN:HB2	4:B:773:HOH:O	2.14	0.47
1:A:305:ALA:O	1:A:308:ALA:HB3	2.14	0.47
1:D:180:VAL:HG13	1:D:222:VAL:HG21	1.96	0.47
1:A:74:ARG:HB3	4:A:540:HOH:O	2.15	0.47
1:D:258:LEU:CD1	1:D:265:GLY:HA3	2.45	0.47
1:D:412:GLN:HG3	1:D:412:GLN:O	2.14	0.47
1:D:377:ALA:O	1:D:381:SER:HB2	2.15	0.47
1:A:332:TYR:C	1:A:334:GLY:H	2.19	0.46
1:A:367:GLY:HA2	1:A:370:THR:O	2.15	0.46
1:B:190:GLN:C	1:B:192:PRO:HD3	2.35	0.46
1:C:336:VAL:C	1:C:338:PRO:HD3	2.35	0.46
1:C:339:GLN:HG3	1:C:340:LYS:N	2.27	0.46
1:C:375:LEU:HD11	1:C:411:GLY:HA3	1.97	0.46
1:C:316:ARG:NH1	1:C:316:ARG:HG3	2.31	0.46
1:C:339:GLN:CG	1:C:340:LYS:N	2.78	0.46
1:C:61:TYR:CE1	1:C:74:ARG:HD2	2.51	0.46
1:C:202:MET:HE1	1:C:219:VAL:CG2	2.45	0.46
1:C:23:GLN:NE2	4:C:568:HOH:O	2.48	0.46
1:D:264:LEU:CD1	1:D:264:LEU:O	2.63	0.46
1:B:336:VAL:HG12	1:B:337:TYR:N	2.31	0.46
1:A:176:ASP:OD1	1:A:215:ARG:NE	2.48	0.46
1:A:326:GLN:HE22	1:A:329:ARG:HH21	1.64	0.46
1:A:243:ILE:CG2	1:A:247:TYR:HB3	2.46	0.46
1:A:287:LEU:HD21	1:A:319:ALA:HB3	1.98	0.46
1:C:267:VAL:O	1:C:271:MET:HG2	2.15	0.46
1:C:330:ARG:HH11	1:C:330:ARG:CB	2.20	0.45
1:C:377:ALA:O	1:C:381:SER:HB2	2.17	0.45
1:B:188:LYS:HE2	1:B:228:LEU:HD22	1.98	0.45
1:C:172:LEU:O	1:C:172:LEU:HD12	2.17	0.45
1:A:109:LEU:HD23	1:A:109:LEU:C	2.37	0.45
1:D:401:ALA:HB3	1:D:402:PRO:HD3	1.99	0.45
1:C:160:HIS:HD2	1:C:163:ASP:OD2	2.00	0.45
1:A:233:GLU:HG2	1:A:234:LYS:H	1.81	0.45
1:B:193:GLU:HG3	4:B:710:HOH:O	2.17	0.45
1:A:232:ASP:OD1	1:A:235:THR:OG1	2.32	0.45
1:D:160:HIS:HB3	1:D:163:ASP:HB2	1.99	0.45
1:C:21:THR:HG22	4:C:624:HOH:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:140:TYR:HA	1:C:141:PRO:HD2	1.85	0.44
1:B:278:ARG:CB	1:B:278:ARG:NH1	2.80	0.44
1:A:175:THR:HA	4:A:526:HOH:O	2.16	0.44
1:D:398:GLN:O	1:D:402:PRO:HD3	2.17	0.44
1:D:26:TYR:HB2	1:D:27:GLN:NE2	2.32	0.44
1:B:202:MET:CE	1:B:219:VAL:CG2	2.87	0.44
1:A:326:GLN:NE2	1:A:329:ARG:HH21	2.15	0.44
1:C:70:ARG:HG3	1:C:70:ARG:HH11	1.83	0.44
1:C:410:GLU:O	1:C:413:ARG:HB3	2.17	0.44
1:B:113:ALA:HB2	1:B:135:TRP:HZ3	1.82	0.44
1:D:323:TYR:O	1:D:327:ILE:HG13	2.18	0.44
1:C:429:THR:HG22	1:D:350:ARG:NH2	2.33	0.44
1:D:328:TYR:CD2	1:D:340:LYS:HB3	2.52	0.44
1:B:342:LEU:O	1:B:346:LEU:HB2	2.18	0.44
1:A:22:ALA:HA	1:A:118:GLN:NE2	2.31	0.44
1:C:160:HIS:HE1	4:C:696:HOH:O	1.99	0.44
1:C:380:PHE:HA	1:C:383:LEU:HB2	2.00	0.44
1:B:304:LYS:HB2	1:C:130:GLN:NE2	2.33	0.44
1:C:73:ALA:HB1	1:C:77:ARG:NH1	2.33	0.44
1:C:78:LEU:O	1:C:78:LEU:HD23	2.18	0.44
1:A:381:SER:HB3	1:A:399:LEU:HD12	2.00	0.44
1:B:108:THR:O	1:B:111:PRO:HD2	2.18	0.44
1:C:177:ILE:HG13	1:C:177:ILE:O	2.18	0.43
1:D:311:GLU:HA	1:D:314:VAL:HG23	2.00	0.43
1:C:244:ALA:N	1:C:245:PRO:CD	2.81	0.43
1:A:356:ALA:O	1:A:360:ILE:HG13	2.19	0.43
1:A:108:THR:C	1:A:111:PRO:HD2	2.38	0.43
1:A:233:GLU:HG2	1:A:234:LYS:N	2.33	0.43
1:C:357:ASP:HB2	4:C:764:HOH:O	2.18	0.43
1:A:404:THR:HG23	1:A:407:GLN:OE1	2.18	0.43
1:A:189:LYS:HB3	1:A:191:GLN:HG3	1.99	0.43
1:B:278:ARG:HD3	1:B:289:LEU:CD2	2.49	0.43
1:B:177:ILE:O	1:B:177:ILE:HG13	2.18	0.43
1:D:381:SER:OG	1:D:396:ALA:HA	2.19	0.43
1:A:353:GLN:NE2	1:A:355:SER:HB2	2.27	0.43
1:D:379:VAL:HG13	1:D:415:VAL:CG2	2.48	0.43
1:D:23:GLN:O	1:D:27:GLN:HG2	2.19	0.43
1:A:267:VAL:O	1:A:271:MET:HG2	2.18	0.43
1:A:331:GLY:HA2	1:A:335:LYS:O	2.19	0.43
1:C:278:ARG:HH11	1:C:278:ARG:HG2	1.83	0.43
1:C:60:THR:CG2	1:C:61:TYR:N	2.81	0.43
1:B:278:ARG:HD3	1:B:289:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:424:THR:O	1:A:424:THR:HG22	2.18	0.42
1:B:115:LEU:HA	4:B:606:HOH:O	2.17	0.42
1:A:110:ILE:N	1:A:111:PRO:CD	2.82	0.42
1:D:35:SER:HG	1:D:38:GLN:CG	2.32	0.42
1:C:69:PRO:HG2	1:C:103:ASN:ND2	2.34	0.42
1:C:82:LYS:HA	1:C:83:PRO:HD3	1.90	0.42
1:D:195:GLN:HA	1:D:195:GLN:OE1	2.20	0.42
1:A:222:VAL:O	1:A:228:LEU:HD12	2.20	0.42
1:A:126:VAL:HG12	1:A:127:ASN:N	2.35	0.42
1:B:54:ILE:HA	1:B:54:ILE:HD13	1.88	0.42
1:B:346:LEU:HD22	1:B:350:ARG:CZ	2.50	0.42
1:D:136:GLN:HB3	1:D:143:ALA:HB1	2.01	0.42
1:C:43:ASP:O	1:C:44:ILE:HG23	2.20	0.42
1:A:331:GLY:HA3	1:A:336:VAL:CG2	2.43	0.41
1:A:112:LEU:HD11	1:A:116:TYR:CZ	2.55	0.41
1:C:237:GLN:O	1:C:241:GLU:HG3	2.21	0.41
1:A:269:GLN:O	1:A:270:MET:C	2.58	0.41
1:D:261:PHE:O	1:D:262:PRO:C	2.58	0.41
1:B:397:THR:HA	1:B:400:GLU:HB3	2.01	0.41
1:D:187:GLN:OE1	1:D:223:LEU:HD22	2.20	0.41
1:B:244:ALA:N	1:B:245:PRO:CD	2.83	0.41
1:D:150:LEU:C	1:D:152:ARG:N	2.73	0.41
1:B:392:ALA:O	1:B:396:ALA:HB2	2.20	0.41
1:A:345:LEU:O	1:A:356:ALA:HB1	2.21	0.41
1:D:391:GLU:N	1:D:391:GLU:CD	2.64	0.41
1:B:150:LEU:C	1:B:150:LEU:HD23	2.40	0.41
1:D:345:LEU:HA	1:D:345:LEU:HD23	1.91	0.41
1:D:316:ARG:HG3	1:D:316:ARG:NH1	2.36	0.41
1:D:267:VAL:O	1:D:271:MET:HG2	2.21	0.41
1:C:296:GLY:HA2	1:C:299:VAL:O	2.20	0.41
1:C:339:GLN:HA	1:D:430:LEU:CB	2.51	0.41
1:B:376:ASN:HA	1:B:379:VAL:HG23	2.02	0.41
1:C:286:GLU:OE1	1:C:309:HIS:CD2	2.73	0.41
1:C:377:ALA:O	1:C:381:SER:CB	2.68	0.41
1:A:259:TYR:CE2	1:A:295:GLU:OE2	2.72	0.41
1:D:133:SER:HA	1:D:136:GLN:HG2	2.02	0.41
1:C:181:GLU:HA	1:C:181:GLU:OE1	2.21	0.41
1:A:339:GLN:O	1:A:343:ASP:HB2	2.21	0.41
1:B:267:VAL:O	1:B:271:MET:HG2	2.21	0.41
1:A:186:TYR:HB2	1:A:195:GLN:HG2	2.02	0.41
1:A:289:LEU:HD22	1:A:309:HIS:CE1	2.56	0.41
1:B:362:GLN:HA	1:B:365:SER:OG	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:248:PRO:C	1:C:250:SER:N	2.74	0.40
1:C:132:ILE:HD12	1:C:150:LEU:HD12	2.02	0.40
1:D:230:THR:HA	1:D:231:PRO:HD2	1.89	0.40
1:D:150:LEU:O	1:D:152:ARG:N	2.54	0.40
1:D:217:ASP:O	1:D:221:ARG:HG3	2.21	0.40
1:C:74:ARG:CZ	1:C:74:ARG:HB2	2.51	0.40
1:B:333:LEU:HA	1:B:333:LEU:HD23	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/452 (86%)	367 (95%)	20 (5%)	0	100	100
1	B	397/452 (88%)	380 (96%)	14 (4%)	3 (1%)	27	46
1	C	397/452 (88%)	372 (94%)	24 (6%)	1 (0%)	50	73
1	D	306/452 (68%)	287 (94%)	17 (6%)	2 (1%)	30	50
All	All	1487/1808 (82%)	1406 (95%)	75 (5%)	6 (0%)	43	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	ALA
1	B	386	ALA
1	C	249	ALA
1	D	151	TYR
1	B	367	GLY
1	D	230	THR

### 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	287/351 (82%)	286 (100%)	1 (0%)	96	99
1	B	287/351 (82%)	283 (99%)	4 (1%)	78	94
1	C	292/351 (83%)	290 (99%)	2 (1%)	91	98
1	D	223/351 (64%)	222 (100%)	1 (0%)	95	99
All	All	1089/1404 (78%)	1081 (99%)	8 (1%)	91	98

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	ARG
1	B	215	ARG
1	B	250	SER
1	B	288	LEU
1	B	346	LEU
1	C	111	PRO
1	C	250	SER
1	D	394	ASP

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

Mol	Chain	Res	Type
1	A	25	ASN
1	A	118	GLN
1	A	154	GLN
1	A	351	ASN
1	A	353	GLN
1	B	160	HIS
1	B	201	GLN
1	B	256	GLN
1	B	309	HIS
1	C	23	GLN
1	C	24	GLN
1	C	125	ASN
1	C	130	GLN

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Mol	Chain	Res	Type
1	C	131	GLN
1	C	187	GLN
1	C	190	GLN
1	C	191	GLN
1	C	195	GLN
1	C	309	HIS
1	C	431	GLN
1	C	433	HIS
1	D	27	GLN
1	D	237	GLN
1	D	276	ASN
1	D	351	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z  > 2$
3	GOL	B	453	-	5,5,5	0.22	0	5,5,5	0.29	0
3	GOL	C	453	-	5,5,5	0.31	0	5,5,5	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	C	455	-	5,5,5	0.28	0	5,5,5	0.27	0
3	GOL	D	453	-	5,5,5	0.15	0	5,5,5	0.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	453	-	-	0/4/4/4	0/0/0/0
3	GOL	C	453	-	-	0/4/4/4	0/0/0/0
3	GOL	C	455	-	-	0/4/4/4	0/0/0/0
3	GOL	D	453	-	-	0/4/4/4	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.

## 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	A	395/452 (87%)	-0.01	4 (1%) 79 81	28, 50, 73, 83	0
1	B	405/452 (89%)	-0.01	11 (2%) 52 54	23, 44, 90, 99	0
1	C	405/452 (89%)	0.10	14 (3%) 42 43	17, 38, 80, 94	0
1	D	316/452 (69%)	0.30	29 (9%) 9 8	26, 52, 84, 95	0
All	All	1521/1808 (84%)	0.08	58 (3%) 38 40	17, 46, 81, 99	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	161	LEU	7.2
1	D	157	TYR	5.6
1	B	429	THR	5.4
1	D	224	GLY	5.1
1	D	399	LEU	4.9
1	B	431	GLN	3.7
1	D	164	VAL	3.7
1	C	357	ASP	3.4
1	C	396	ALA	3.2
1	D	143	ALA	3.2
1	D	148	VAL	3.2
1	C	397	THR	3.1
1	D	140	TYR	3.0
1	D	150	LEU	2.9
1	C	358	PHE	2.9
1	B	430	LEU	2.8
1	C	379	VAL	2.7
1	C	365	SER	2.7
1	D	135	TRP	2.7
1	B	395	LEU	2.7
1	D	26	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	413	ARG	2.7
1	D	159	GLN	2.6
1	C	372	PRO	2.5
1	D	392	ALA	2.5
1	B	396	ALA	2.5
1	A	430	LEU	2.5
1	D	186	TYR	2.5
1	C	383	LEU	2.5
1	C	375	LEU	2.4
1	D	223	LEU	2.4
1	D	160	HIS	2.4
1	D	192	PRO	2.4
1	D	162	ASP	2.4
1	D	136	GLN	2.4
1	B	397	THR	2.3
1	A	293	TYR	2.3
1	D	29	LEU	2.3
1	B	402	PRO	2.3
1	D	27	GLN	2.3
1	D	163	ASP	2.2
1	D	151	TYR	2.2
1	C	346	LEU	2.2
1	B	378	TYR	2.2
1	A	228	LEU	2.2
1	B	403	LEU	2.2
1	C	342	LEU	2.2
1	B	392	ALA	2.2
1	D	152	ARG	2.1
1	D	396	ALA	2.1
1	D	185	VAL	2.1
1	C	420	ALA	2.1
1	B	375	LEU	2.1
1	D	147	GLN	2.0
1	C	377	ALA	2.0
1	D	257	LEU	2.0
1	D	395	LEU	2.0
1	A	90	HIS	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	453	6/6	0.21	7.17	60,61,62,64	0
3	GOL	C	455	6/6	0.25	4.28	71,72,72,73	0
3	GOL	D	453	6/6	0.19	1.17	70,70,71,72	0
3	GOL	C	453	6/6	0.13	0.26	50,52,53,55	0
2	CL	C	454	1/1	0.14	-0.55	51,51,51,51	0
2	CL	B	454	1/1	0.12	-0.87	82,82,82,82	0
2	CL	A	453	1/1	0.07	-1.55	66,66,66,66	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.