



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 10:46 pm BST

PDB ID : 3BP8  
Title : Crystal structure of Mlc/EIIB complex  
Authors : An, Y.J.; Jung, H.I.; Cha, S.S.  
Deposited on : 2007-12-18  
Resolution : 2.85 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

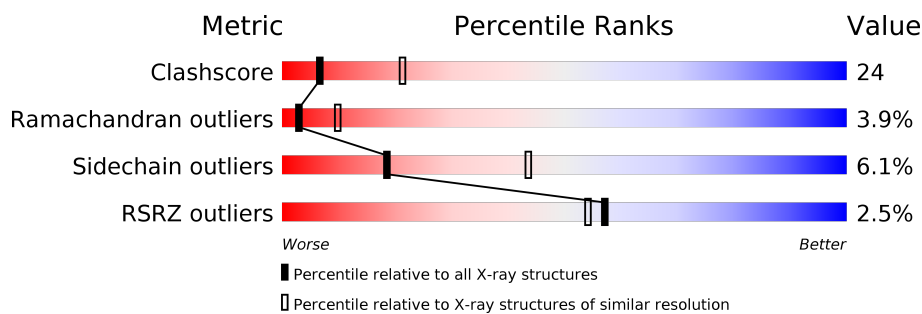
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	406	<div> <div>%</div> <div> <div></div> <div>49%</div> <div>40%</div> <div>6%</div> </div> </div>
1	B	406	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>39%</div> <div>6%</div> </div> </div>
2	C	75	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>39%</div> </div> </div>
2	D	75	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>35%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6943 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.

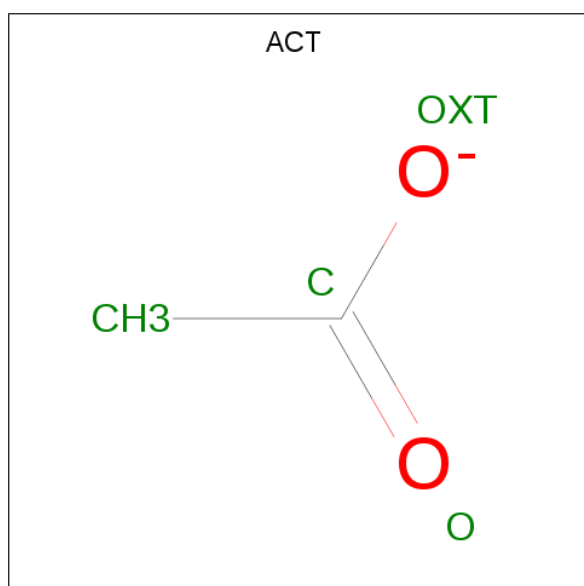
- Molecule 1 is a protein called Putative NAGC-like transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	71	0	0
			2927	1849	514	552	12			
1	B	380	Total	C	N	O	S	160	0	0
			2918	1846	512	547	13			

- Molecule 2 is a protein called PTS system glucose-specific EIICB component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	75	Total	C	N	O	S	30	0	0
			542	338	95	106	3			
2	D	75	Total	C	N	O	S	34	0	0
			542	338	95	106	3			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

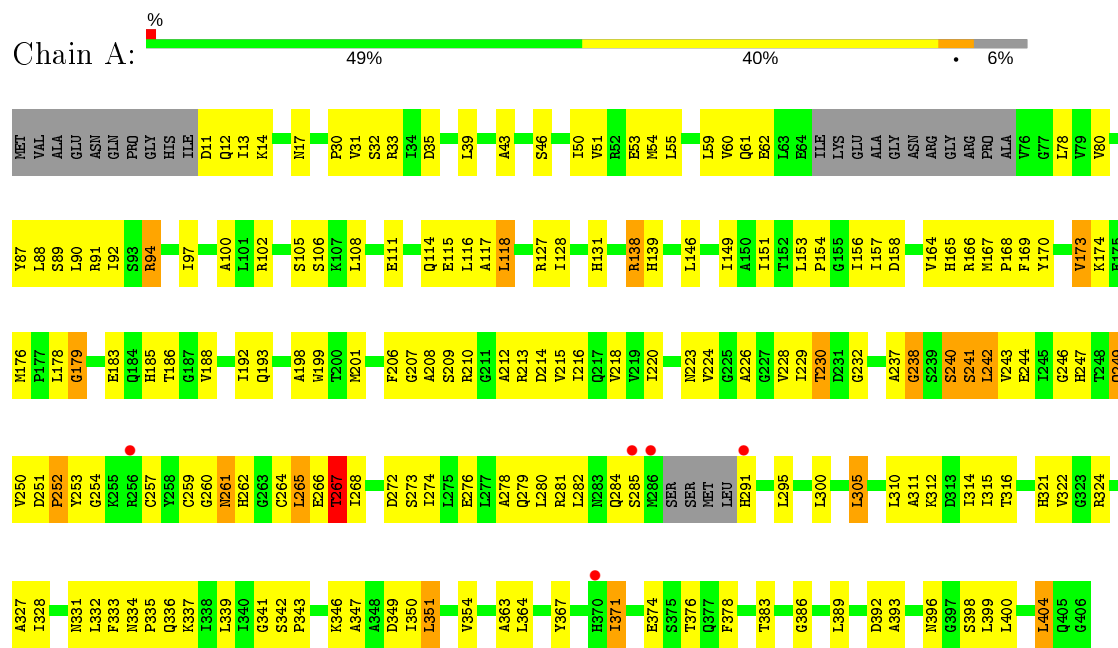
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	A	1	Total Zn 1 1	0	0

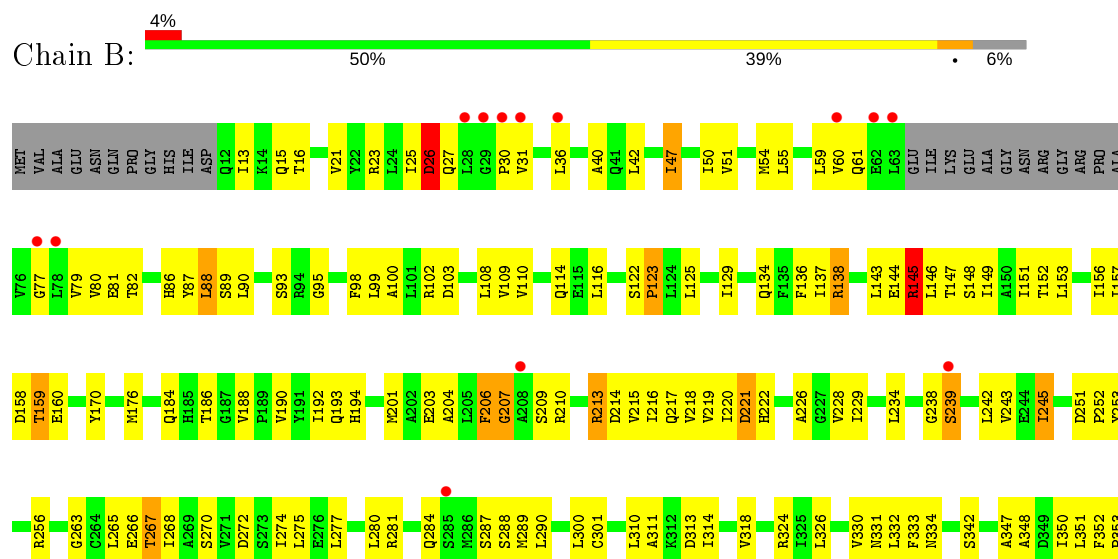
### 3 Residue-property plots

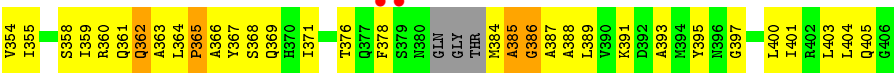
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Putative NAGC-like transcriptional regulator

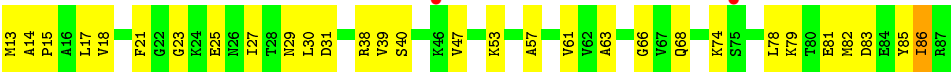


- Molecule 1: Putative NAGC-like transcriptional regulator

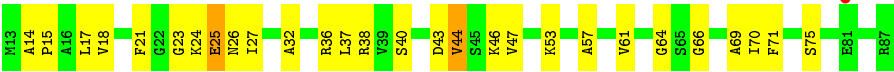




● Molecule 2: PTS system glucose-specific EIICB component



● Molecule 2: PTS system glucose-specific EIICB component



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.43 Å   55.42 Å   82.46 Å 90.00°   95.29°   90.00°	Depositor
Resolution (Å)	20.00 – 2.85 30.01 – 2.82	Depositor EDS
% Data completeness (in resolution range)	83.2 (20.00-2.85) 90.9 (30.01-2.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.80 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.228   ,   0.301 0.237   ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23   ,   25.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ACT

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	0.47	0/2972	0.71	1/4026 (0.0%)
1	B	0.44	0/2963	0.65	0/4013
2	C	0.51	0/545	0.67	0/732
2	D	0.41	0/545	0.57	0/732
All	All	0.46	0/7025	0.67	1/9503 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	SER	N-CA-C	-5.12	97.18	111.00

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	A	2927	0	2976	138	0
1	B	2918	0	2978	145	0
2	C	542	0	563	24	0
2	D	542	0	563	27	0
3	A	12	0	9	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
All	All	6943	0	7089	313	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 24.

All (313) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLU:HB3	1:A:404:LEU:HD21	1.38	1.03
1:B:193:GLN:HB2	1:B:389:LEU:HD21	1.53	0.91
1:A:100:ALA:HB2	1:A:111:GLU:HG3	1.51	0.90
1:B:267:THR:HG22	1:B:268:ILE:HD12	1.52	0.90
1:B:157:ILE:HG21	1:B:192:ILE:HG21	1.58	0.83
1:B:21:VAL:HG21	1:B:50:ILE:HG21	1.62	0.82
1:B:79:VAL:HG22	1:B:80:VAL:H	1.44	0.82
1:B:314:ILE:O	1:B:318:VAL:HG23	1.78	0.81
1:A:214:ASP:HA	1:A:229:ILE:O	1.83	0.77
1:B:355:ILE:O	1:B:359:ILE:HG13	1.83	0.77
1:A:108:LEU:HD23	1:A:108:LEU:H	1.50	0.76
2:D:32:ALA:HB2	2:D:37:LEU:HD12	1.67	0.74
1:A:305:LEU:HD21	1:A:347:ALA:HA	1.69	0.74
1:B:288:SER:C	1:B:290:LEU:H	1.89	0.74
1:B:148:SER:HA	1:B:188:VAL:HB	1.70	0.74
1:B:267:THR:HG22	1:B:268:ILE:CD1	2.17	0.73
1:B:216:ILE:HD12	1:B:228:VAL:HG22	1.71	0.71
1:A:146:LEU:HD22	2:C:63:ALA:HB2	1.71	0.71
2:C:18:VAL:HG12	2:C:23:GLY:HA2	1.72	0.71
1:A:178:LEU:HD13	1:A:178:LEU:O	1.90	0.70
1:B:204:ALA:O	1:B:210:ARG:HA	1.91	0.70
1:B:358:SER:O	1:B:362:GLN:HG3	1.89	0.70
1:B:216:ILE:CD1	1:B:228:VAL:HG22	2.21	0.70
1:A:59:LEU:HD13	1:A:400:LEU:HD12	1.72	0.70
1:B:252:PRO:HG2	1:B:253:TYR:CE1	2.26	0.70
1:B:352:PHE:HB2	1:B:353:PRO:HD3	1.74	0.69
1:A:350:ILE:HD12	1:A:350:ILE:N	2.08	0.68
2:D:14:ALA:N	2:D:15:PRO:HD2	2.09	0.68
1:B:61:GLN:HG3	1:B:81:GLU:HB2	1.76	0.68
2:C:82:MET:O	2:C:86:ILE:HG12	1.93	0.68
1:A:267:THR:HG22	1:A:268:ILE:HG13	1.76	0.68
1:A:300:LEU:HD23	1:A:311:ALA:HB1	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HA	1:B:243:VAL:HG13	1.76	0.68
1:A:331:ASN:HD21	1:A:363:ALA:HA	1.59	0.67
1:B:55:LEU:HD23	1:B:60:VAL:HG23	1.76	0.67
1:B:203:GLU:HA	1:B:207:GLY:HA3	1.77	0.67
2:D:14:ALA:O	2:D:18:VAL:HG23	1.95	0.66
1:A:214:ASP:H	1:A:336:GLN:HE22	1.41	0.66
1:A:105:SER:O	1:A:106:SER:HB2	1.96	0.66
2:C:18:VAL:HG21	2:C:85:TYR:CD2	2.31	0.66
1:B:216:ILE:HG21	1:B:326:LEU:HD11	1.78	0.65
1:B:300:LEU:HD23	1:B:311:ALA:HB1	1.78	0.65
2:C:15:PRO:HB3	2:C:85:TYR:CE1	2.31	0.65
1:B:386:GLY:O	1:B:388:ALA:N	2.30	0.64
1:B:88:LEU:HD11	1:B:99:LEU:HD23	1.80	0.64
1:A:158:ASP:HB2	1:A:165:HIS:NE2	2.11	0.64
1:B:266:GLU:O	1:B:270:SER:HB2	1.98	0.64
1:B:50:ILE:O	1:B:54:MET:HG3	1.97	0.64
1:A:193:GLN:HB2	1:A:389:LEU:HD21	1.80	0.63
2:C:29:ASN:HB3	2:C:40:SER:HB2	1.79	0.63
1:A:115:GLU:O	1:A:116:LEU:HG	1.99	0.63
1:B:50:ILE:O	1:B:54:MET:HE2	1.99	0.63
1:A:13:ILE:O	1:A:17:ASN:HB2	1.99	0.62
2:C:18:VAL:HG21	2:C:85:TYR:HD2	1.63	0.62
1:B:152:THR:HA	1:B:193:GLN:O	1.99	0.62
1:B:213:ARG:HH11	1:B:213:ARG:HB3	1.65	0.62
1:B:158:ASP:O	1:B:160:GLU:N	2.30	0.62
1:B:275:LEU:HD23	1:B:300:LEU:HD12	1.82	0.61
1:B:86:HIS:HD2	1:B:144:GLU:H	1.48	0.61
1:B:157:ILE:HG22	1:B:159:THR:H	1.66	0.61
2:D:14:ALA:N	2:D:15:PRO:CD	2.63	0.61
1:A:117:ALA:O	1:A:118:LEU:HB3	2.01	0.61
1:B:203:GLU:OE1	1:B:376:THR:HB	2.00	0.61
1:A:157:ILE:HG21	1:A:192:ILE:HG22	1.83	0.60
1:A:153:LEU:HD23	1:A:153:LEU:N	2.15	0.60
1:A:278:ALA:HB3	1:A:295:LEU:HD21	1.84	0.59
1:A:179:GLY:O	1:A:183:GLU:HB2	2.01	0.59
2:C:61:VAL:HB	2:C:68:GLN:HB2	1.85	0.59
1:B:36:LEU:O	1:B:40:ALA:HB3	2.03	0.59
1:A:108:LEU:N	1:A:108:LEU:HD23	2.15	0.59
1:A:54:MET:HE3	1:A:400:LEU:HD21	1.85	0.59
1:A:247:HIS:CD2	1:B:364:LEU:HD23	2.38	0.59
1:A:12:GLN:HG2	1:A:13:ILE:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:TYR:HE1	1:A:89:SER:HB2	1.68	0.58
2:C:30:LEU:HD22	2:C:79:LYS:HG2	1.84	0.58
1:B:116:LEU:HD23	1:B:170:TYR:OH	2.03	0.58
2:D:36:ARG:CD	2:D:70:ILE:HG12	2.34	0.58
1:B:25:ILE:O	1:B:26:ASP:HB3	2.01	0.58
1:B:350:ILE:O	1:B:354:VAL:HG23	2.04	0.58
1:B:59:LEU:HD13	1:B:400:LEU:HD11	1.86	0.58
1:B:61:GLN:HB2	1:B:79:VAL:CG1	2.34	0.57
1:A:87:TYR:CE1	1:A:89:SER:HB2	2.39	0.57
1:A:310:LEU:O	1:A:310:LEU:HD23	2.04	0.57
1:A:241:SER:OG	1:B:367:TYR:CE1	2.57	0.57
1:B:384:MET:O	1:B:385:ALA:HB3	2.05	0.57
1:B:125:LEU:O	1:B:129:ILE:HG13	2.05	0.57
1:B:86:HIS:CD2	1:B:144:GLU:H	2.22	0.57
1:A:278:ALA:O	1:A:282:LEU:HG	2.04	0.57
1:B:288:SER:O	1:B:290:LEU:N	2.38	0.56
1:B:280:LEU:O	1:B:284:GLN:HG3	2.06	0.56
1:B:61:GLN:HB2	1:B:79:VAL:HG13	1.86	0.56
1:A:218:VAL:HA	1:A:226:ALA:CB	2.35	0.56
1:A:237:ALA:HB3	1:A:241:SER:O	2.06	0.56
1:A:315:ILE:HG23	1:A:351:LEU:HG	1.88	0.56
1:B:13:ILE:HD12	1:B:13:ILE:H	1.71	0.56
1:B:288:SER:C	1:B:290:LEU:N	2.58	0.56
1:B:360:ARG:HG2	1:B:368:SER:HB2	1.88	0.56
1:A:157:ILE:HD12	1:A:164:VAL:HG22	1.88	0.56
1:B:220:ILE:HB	1:B:342:SER:HB2	1.86	0.56
2:D:53:LYS:HA	2:D:57:ALA:HB3	1.86	0.56
1:A:108:LEU:CD2	1:A:108:LEU:H	2.18	0.55
1:B:122:SER:O	1:B:123:PRO:O	2.24	0.55
1:B:245:ILE:O	1:B:245:ILE:HD13	2.06	0.55
1:B:145:ARG:HD3	2:D:36:ARG:CG	2.36	0.55
2:C:17:LEU:HD11	2:C:78:LEU:HD13	1.89	0.55
1:A:218:VAL:HA	1:A:226:ALA:HB2	1.89	0.55
1:B:206:PHE:HA	1:B:210:ARG:HE	1.70	0.55
1:B:274:ILE:HG23	1:B:314:ILE:CG2	2.37	0.55
1:A:90:LEU:O	1:A:151:ILE:HA	2.06	0.54
1:B:88:LEU:HD11	1:B:99:LEU:CD2	2.38	0.54
2:D:69:ALA:HB1	2:D:71:PHE:HE1	1.72	0.54
1:B:143:LEU:HD23	1:B:145:ARG:H	1.73	0.54
1:A:310:LEU:O	1:A:314:ILE:HG12	2.07	0.54
1:A:138:ARG:HD3	1:A:139:HIS:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLY:HA2	1:A:376:THR:HG21	1.89	0.54
1:B:288:SER:HB2	1:B:310:LEU:HD22	1.89	0.54
1:A:216:ILE:HG13	1:A:335:PRO:HG3	1.89	0.54
1:B:79:VAL:HG22	1:B:80:VAL:N	2.19	0.54
1:A:153:LEU:HD12	1:A:167:MET:SD	2.47	0.53
1:B:51:VAL:HA	1:B:54:MET:HE2	1.90	0.53
1:A:214:ASP:HB2	1:A:335:PRO:HA	1.90	0.53
1:A:264:CYS:O	1:A:265:LEU:C	2.46	0.53
1:B:146:LEU:HB3	2:D:61:VAL:HG11	1.90	0.53
2:D:36:ARG:HD2	2:D:70:ILE:HG12	1.90	0.53
1:B:87:TYR:HE1	1:B:89:SER:HB3	1.73	0.53
2:C:78:LEU:O	2:C:82:MET:HG3	2.09	0.53
1:A:279:GLN:C	1:A:281:ARG:H	2.11	0.53
1:A:32:SER:HB3	1:A:35:ASP:OD2	2.08	0.53
2:D:69:ALA:HB1	2:D:71:PHE:CE1	2.44	0.53
1:A:242:LEU:HD23	1:A:242:LEU:H	1.73	0.52
1:B:186:THR:O	2:D:61:VAL:HA	2.09	0.52
1:B:333:PHE:O	1:B:334:ASN:C	2.48	0.52
1:A:170:TYR:O	1:A:173:VAL:HG22	2.09	0.52
1:B:301:CYS:HB3	1:B:347:ALA:HB2	1.90	0.52
1:A:185:HIS:CG	1:A:185:HIS:O	2.63	0.52
2:C:30:LEU:CD2	2:C:79:LYS:HG2	2.40	0.52
1:B:226:ALA:HB3	1:B:245:ILE:HG21	1.91	0.52
1:A:279:GLN:O	1:A:281:ARG:N	2.43	0.52
1:A:176:MET:HG2	1:A:178:LEU:HB2	1.92	0.52
1:B:215:VAL:HG12	1:B:216:ILE:N	2.25	0.52
1:A:90:LEU:HD21	1:A:151:ILE:HG12	1.92	0.51
1:B:193:GLN:NE2	1:B:242:LEU:HD22	2.25	0.51
1:B:326:LEU:O	1:B:330:VAL:HG23	2.11	0.51
1:A:371:ILE:HG23	1:A:371:ILE:O	2.11	0.51
1:B:59:LEU:HD13	1:B:400:LEU:CD1	2.41	0.51
1:A:249:GLN:HB3	1:B:362:GLN:HB3	1.92	0.51
1:A:252:PRO:HG2	1:A:253:TYR:CE1	2.46	0.51
1:A:312:LYS:HG3	1:A:350:ILE:HG21	1.93	0.51
1:A:364:LEU:HD11	1:B:156:ILE:HD12	1.93	0.51
1:B:203:GLU:HG3	1:B:217:GLN:HE22	1.75	0.51
1:A:30:PRO:HA	1:A:78:LEU:O	2.10	0.50
1:B:209:SER:HB2	1:B:215:VAL:HG21	1.94	0.50
1:A:94:ARG:HG2	1:A:94:ARG:O	2.11	0.50
1:B:384:MET:O	1:B:385:ALA:CB	2.60	0.50
1:B:30:PRO:HB2	1:B:77:GLY:CA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:NH2	1:A:383:THR:OG1	2.34	0.49
1:B:400:LEU:O	1:B:404:LEU:HG	2.11	0.49
2:C:79:LYS:O	2:C:83:ASP:HB2	2.12	0.49
1:A:212:ALA:HB1	1:A:336:GLN:HE21	1.77	0.49
1:A:35:ASP:O	1:A:39:LEU:HG	2.13	0.49
1:A:117:ALA:O	1:A:118:LEU:CB	2.60	0.49
1:A:230:THR:C	1:A:232:GLY:H	2.15	0.49
1:A:92:ILE:HD13	1:A:128:ILE:HD13	1.95	0.49
1:A:206:PHE:O	1:A:378:PHE:CE1	2.66	0.49
1:B:15:GLN:O	1:B:397:GLY:HA3	2.13	0.49
1:B:147:THR:HG22	1:B:403:LEU:HD11	1.95	0.48
1:A:127:ARG:HG2	1:A:131:HIS:HE1	1.78	0.48
1:A:350:ILE:HD12	1:A:350:ILE:H	1.77	0.48
1:B:143:LEU:HD23	1:B:144:GLU:N	2.27	0.48
1:B:15:GLN:HB2	1:B:401:ILE:HD12	1.95	0.48
1:B:238:GLY:O	1:B:239:SER:CB	2.60	0.48
2:D:57:ALA:HA	2:D:70:ILE:O	2.14	0.48
1:B:218:VAL:HG21	1:B:326:LEU:HD22	1.95	0.48
1:B:143:LEU:HD23	1:B:145:ARG:N	2.28	0.48
1:B:108:LEU:HD23	1:B:109:VAL:N	2.29	0.48
1:B:389:LEU:HD12	1:B:389:LEU:H	1.79	0.47
1:B:251:ASP:O	1:B:263:GLY:HA3	2.14	0.47
2:D:37:LEU:HB3	2:D:69:ALA:HB3	1.95	0.47
1:A:207:GLY:H	1:A:210:ARG:NE	2.13	0.47
1:B:134:GLN:O	1:B:137:ILE:HG12	2.14	0.47
1:B:21:VAL:O	1:B:25:ILE:HG13	2.15	0.47
1:A:220:ILE:O	1:A:342:SER:HB2	2.14	0.47
1:A:156:ILE:HD12	1:A:166:ARG:HD3	1.95	0.47
1:A:237:ALA:HB1	1:B:334:ASN:HB3	1.97	0.47
1:B:136:PHE:HB3	2:D:64:GLY:HA3	1.96	0.47
1:B:274:ILE:HG23	1:B:314:ILE:HG21	1.97	0.47
1:B:15:GLN:HB2	1:B:401:ILE:CD1	2.45	0.47
2:D:43:ASP:OD2	2:D:46:LYS:HG3	2.14	0.47
1:B:137:ILE:HG13	1:B:138:ARG:N	2.29	0.47
1:B:93:SER:HB3	1:B:98:PHE:HE1	1.80	0.47
1:A:324:ARG:O	1:A:327:ALA:HB3	2.14	0.47
1:A:168:PRO:O	1:A:169:PHE:HB2	2.14	0.46
1:A:11:ASP:HB3	1:A:14:LYS:HB3	1.97	0.46
1:A:224:VAL:H	1:A:266:GLU:HG3	1.79	0.46
1:A:244:GLU:C	1:A:246:GLY:H	2.18	0.46
1:A:343:PRO:O	1:A:346:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HG23	1:A:314:ILE:CG2	2.44	0.46
1:B:80:VAL:HG22	1:B:82:THR:HG23	1.97	0.46
1:A:90:LEU:N	1:A:90:LEU:HD23	2.30	0.46
1:B:60:VAL:HA	1:B:80:VAL:HA	1.98	0.46
1:B:145:ARG:HD3	2:D:36:ARG:HG2	1.97	0.46
1:B:145:ARG:HD3	2:D:36:ARG:HG3	1.97	0.46
1:B:157:ILE:HG21	1:B:192:ILE:CG2	2.40	0.46
1:A:168:PRO:O	1:A:169:PHE:CB	2.64	0.45
1:A:367:TYR:OH	1:B:242:LEU:O	2.29	0.45
1:B:220:ILE:HB	1:B:342:SER:CB	2.45	0.45
1:B:365:PRO:O	1:B:367:TYR:N	2.49	0.45
1:A:209:SER:HB3	1:A:339:LEU:HD11	1.97	0.45
1:B:352:PHE:CD2	1:B:352:PHE:N	2.84	0.45
1:A:244:GLU:HG2	1:B:364:LEU:HG	1.99	0.45
2:C:40:SER:HA	2:C:66:GLY:HA2	1.99	0.45
1:B:216:ILE:CG2	1:B:326:LEU:HD11	2.45	0.45
1:A:240:SER:O	1:A:241:SER:C	2.55	0.45
1:A:284:GLN:O	1:A:285:SER:HB3	2.16	0.44
1:B:203:GLU:HG3	1:B:217:GLN:NE2	2.31	0.44
1:B:30:PRO:HB2	1:B:77:GLY:HA3	1.99	0.44
1:A:213:ARG:O	1:A:229:ILE:HG22	2.17	0.44
1:A:55:LEU:HD21	1:A:62:GLU:HG3	1.98	0.44
1:B:125:LEU:HD12	1:B:176:MET:HG3	1.98	0.44
1:B:331:ASN:HD21	1:B:363:ALA:HA	1.82	0.44
1:A:154:PRO:O	1:A:167:MET:HG3	2.17	0.44
1:B:100:ALA:HA	1:B:110:VAL:O	2.17	0.44
1:A:237:ALA:C	1:A:241:SER:HB3	2.38	0.44
1:B:13:ILE:HA	1:B:16:THR:HG22	1.99	0.44
1:A:247:HIS:CG	1:B:364:LEU:HD23	2.53	0.44
1:A:324:ARG:HH22	1:B:324:ARG:HG2	1.83	0.44
1:A:193:GLN:HB3	1:A:198:ALA:HB2	2.00	0.44
1:B:151:ILE:CD1	1:B:190:VAL:HG13	2.48	0.44
1:B:364:LEU:HB3	1:B:367:TYR:CD2	2.53	0.44
1:B:360:ARG:NH2	1:B:371:ILE:O	2.50	0.44
2:C:21:PHE:HA	2:C:47:VAL:HG13	1.99	0.44
1:A:244:GLU:C	1:A:246:GLY:N	2.71	0.44
1:A:59:LEU:HD13	1:A:400:LEU:CD1	2.45	0.44
1:A:60:VAL:HG12	1:A:61:GLN:N	2.32	0.44
1:A:97:ILE:HG23	1:A:114:GLN:HB2	2.00	0.43
1:B:221:ASP:HB3	1:B:222:HIS:H	1.32	0.43
1:B:391:LYS:HB3	1:B:395:TYR:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASN:OD1	1:A:396:ASN:C	2.56	0.43
1:A:51:VAL:HG11	1:A:78:LEU:HD21	2.00	0.43
1:A:215:VAL:O	1:A:228:VAL:HA	2.19	0.43
1:B:193:GLN:HG3	1:B:194:HIS:N	2.33	0.43
1:B:23:ARG:O	1:B:27:GLN:NE2	2.43	0.43
1:A:272:ASP:O	1:A:276:GLU:HG3	2.18	0.43
1:B:102:ARG:HH21	1:B:385:ALA:HB2	1.83	0.43
1:A:169:PHE:CZ	1:A:223:ASN:ND2	2.86	0.43
1:A:243:VAL:HG13	1:B:332:LEU:HD23	2.01	0.43
1:B:348:ALA:C	1:B:350:ILE:H	2.21	0.43
1:B:348:ALA:O	1:B:353:PRO:HD3	2.19	0.43
1:A:186:THR:OG1	1:A:188:VAL:HG22	2.19	0.43
1:A:393:ALA:HA	1:A:396:ASN:ND2	2.34	0.43
2:C:27:ILE:HG23	2:C:39:VAL:CG2	2.49	0.43
1:A:261:ASN:HB3	1:A:262:HIS:H	1.72	0.43
1:A:97:ILE:CG2	1:A:114:GLN:HB2	2.48	0.43
1:A:259:CYS:SG	1:A:260:GLY:N	2.91	0.43
1:B:324:ARG:HA	1:B:362:GLN:NE2	2.34	0.42
2:C:14:ALA:N	2:C:15:PRO:HD2	2.33	0.42
2:D:36:ARG:O	2:D:75:SER:HB3	2.19	0.42
2:D:44:VAL:HA	2:D:47:VAL:HG23	2.01	0.42
2:C:31:ASP:O	2:C:38:ARG:O	2.36	0.42
1:A:43:ALA:HB3	1:A:46:SER:CB	2.48	0.42
1:A:216:ILE:HG23	1:A:228:VAL:HG12	2.00	0.42
1:A:316:THR:HG23	1:A:354:VAL:HG21	2.02	0.42
1:A:321:HIS:O	1:A:322:VAL:C	2.55	0.42
1:A:151:ILE:HB	1:A:192:ILE:HG12	2.01	0.42
1:A:337:LYS:HD3	1:A:374:GLU:OE2	2.19	0.42
1:B:216:ILE:HG21	1:B:326:LEU:CD1	2.49	0.42
2:D:26:ASN:HD21	2:D:43:ASP:HB3	1.84	0.42
1:A:88:LEU:HD12	1:A:100:ALA:O	2.20	0.42
2:D:23:GLY:O	2:D:25:GLU:N	2.53	0.42
1:A:209:SER:HA	1:A:337:LYS:HD2	2.02	0.42
1:A:199:TRP:HZ2	1:A:378:PHE:O	2.03	0.42
1:B:214:ASP:HA	1:B:229:ILE:O	2.19	0.42
1:B:389:LEU:O	1:B:393:ALA:HB2	2.19	0.42
1:B:109:VAL:O	1:B:110:VAL:HG13	2.20	0.41
2:D:17:LEU:O	2:D:21:PHE:HD2	2.03	0.41
1:B:15:GLN:HG3	1:B:397:GLY:C	2.41	0.41
1:A:392:ASP:O	1:A:396:ASN:ND2	2.53	0.41
1:B:42:LEU:CB	1:B:47:ILE:HB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HB3	1:B:149:ILE:HG13	2.02	0.41
2:D:14:ALA:H	2:D:15:PRO:CD	2.33	0.41
1:B:277:LEU:CD1	1:B:281:ARG:HH21	2.34	0.41
1:A:193:GLN:HE22	1:A:201:MET:CE	2.34	0.41
1:A:273:SER:O	1:A:276:GLU:N	2.52	0.41
1:A:33:ARG:H	1:A:33:ARG:HG2	1.74	0.41
1:B:15:GLN:HA	1:B:401:ILE:HD11	2.03	0.41
2:D:21:PHE:HB2	2:D:27:ILE:HD11	2.02	0.41
2:D:40:SER:HA	2:D:66:GLY:HA2	2.03	0.41
1:B:25:ILE:HG12	1:B:36:LEU:HD21	2.02	0.41
2:D:57:ALA:HB2	2:D:71:PHE:CE1	2.56	0.41
1:B:25:ILE:HG13	1:B:25:ILE:H	1.75	0.41
1:B:277:LEU:HD11	1:B:281:ARG:HH21	1.85	0.41
1:A:230:THR:O	1:A:232:GLY:N	2.48	0.41
1:A:333:PHE:O	1:A:334:ASN:HB3	2.21	0.41
1:A:386:GLY:HA2	1:A:389:LEU:HD12	2.03	0.41
2:C:29:ASN:O	2:C:39:VAL:HG23	2.21	0.41
1:A:146:LEU:CD2	2:C:63:ALA:HB2	2.46	0.41
1:A:92:ILE:O	1:A:154:PRO:HD2	2.21	0.41
1:B:90:LEU:HD12	1:B:151:ILE:HG23	2.03	0.41
1:B:219:VAL:C	1:B:220:ILE:HG13	2.41	0.41
1:A:251:ASP:HA	1:A:252:PRO:HD2	1.92	0.40
2:C:39:VAL:O	2:C:39:VAL:HG13	2.20	0.40
1:A:257:CYS:HB3	1:A:259:CYS:SG	2.61	0.40
1:A:188:VAL:HG13	2:C:61:VAL:HG13	2.03	0.40
1:A:252:PRO:HG2	1:A:253:TYR:CD1	2.57	0.40
1:B:201:MET:HB2	1:B:234:LEU:HD13	2.02	0.40
1:A:305:LEU:CD2	1:A:347:ALA:HA	2.46	0.40
1:A:206:PHE:O	1:A:378:PHE:CZ	2.75	0.40
1:A:46:SER:O	1:A:50:ILE:HG13	2.22	0.40
1:A:237:ALA:HB1	1:B:333:PHE:O	2.21	0.40
1:B:87:TYR:CE2	1:B:102:ARG:HB2	2.57	0.40
2:C:53:LYS:HA	2:C:57:ALA:HB3	2.04	0.40
2:C:79:LYS:HD3	2:C:79:LYS:C	2.42	0.40
1:A:237:ALA:O	1:A:238:GLY:C	2.60	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	375/406 (92%)	313 (84%)	45 (12%)	17 (4%)	2	7
1	B	374/406 (92%)	310 (83%)	50 (13%)	14 (4%)	3	11
2	C	73/75 (97%)	62 (85%)	9 (12%)	2 (3%)	5	16
2	D	73/75 (97%)	63 (86%)	8 (11%)	2 (3%)	5	16
All	All	895/962 (93%)	748 (84%)	112 (12%)	35 (4%)	3	10

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ALA
1	A	249	GLN
1	A	280	LEU
1	B	26	ASP
1	B	123	PRO
2	D	38	ARG
1	A	118	LEU
1	A	174	LYS
1	A	238	GLY
1	A	241	SER
1	A	254	GLY
1	A	261	ASN
1	B	145	ARG
1	B	159	THR
1	B	289	MET
1	B	385	ALA
1	B	386	GLY
1	B	387	ALA
1	A	94	ARG
1	A	252	PRO
1	A	398	SER
1	A	399	LEU

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Mol	Chain	Res	Type
1	B	206	PHE
1	B	207	GLY
1	B	366	ALA
1	A	267	THR
1	A	371	ILE
2	D	24	LYS
1	A	179	GLY
1	B	365	PRO
2	C	74	LYS
1	A	80	VAL
1	B	47	ILE
1	B	95	GLY
2	C	86	ILE

### 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	320/339 (94%)	304 (95%)	16 (5%)	24	53
1	B	320/339 (94%)	295 (92%)	25 (8%)	12	32
2	C	56/56 (100%)	53 (95%)	3 (5%)	22	49
2	D	56/56 (100%)	54 (96%)	2 (4%)	35	66
All	All	752/790 (95%)	706 (94%)	46 (6%)	18	43

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	91	ARG
1	A	138	ARG
1	A	149	ILE
1	A	173	VAL
1	A	230	THR
1	A	242	LEU
1	A	250	VAL

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Mol	Chain	Res	Type
1	A	265	LEU
1	A	267	THR
1	A	291	HIS
1	A	305	LEU
1	A	328	ILE
1	A	349	ASP
1	A	351	LEU
1	A	404	LEU
1	B	26	ASP
1	B	31	VAL
1	B	88	LEU
1	B	103	ASP
1	B	114	GLN
1	B	138	ARG
1	B	145	ARG
1	B	153	LEU
1	B	184	GLN
1	B	213	ARG
1	B	221	ASP
1	B	239	SER
1	B	245	ILE
1	B	256	ARG
1	B	265	LEU
1	B	267	THR
1	B	272	ASP
1	B	287	SER
1	B	313	ASP
1	B	351	LEU
1	B	361	GLN
1	B	362	GLN
1	B	369	GLN
1	B	378	PHE
1	B	405	GLN
2	C	13	MET
2	C	25	GLU
2	C	81	GLU
2	D	25	GLU
2	D	44	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	134	GLN
1	A	139	HIS
1	A	193	GLN
1	A	334	ASN
1	A	336	GLN
1	A	380	ASN
1	B	86	HIS
1	B	114	GLN
1	B	134	GLN
1	B	184	GLN
1	B	193	GLN
1	B	334	ASN
1	B	405	GLN
2	D	26	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	ACT	A	409	-	1,3,3	3.44	1 (100%)	0,3,3	0.00	-
3	ACT	A	407	-	1,3,3	3.44	1 (100%)	0,3,3	0.00	-
3	ACT	A	408	-	1,3,3	3.51	1 (100%)	0,3,3	0.00	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	408	ACT	CH3-C	3.51	1.53	1.48
3	A	407	ACT	CH3-C	3.44	1.53	1.48
3	A	409	ACT	CH3-C	3.44	1.53	1.48

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 [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	381/406 (93%)	-0.14	5 (1%) 77 76	12, 38, 60, 74	19 (4%)
1	B	380/406 (93%)	-0.04	15 (3%) 39 34	18, 46, 80, 93	42 (11%)
2	C	75/75 (100%)	-0.22	2 (2%) 54 50	24, 35, 43, 53	7 (9%)
2	D	75/75 (100%)	-0.01	1 (1%) 77 76	38, 57, 79, 87	8 (10%)
All	All	911/962 (94%)	-0.09	23 (2%) 57 54	12, 42, 73, 93	76 (8%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	LEU	5.0
1	B	78	LEU	4.5
1	A	286	MET	3.5
1	B	62	GLU	3.4
1	B	77	GLY	3.3
1	B	30	PRO	3.2
1	B	239	SER	3.1
1	A	285	SER	2.9
1	B	285	SER	2.7
1	A	256	ARG	2.6
1	B	208	ALA	2.5
1	A	370	HIS	2.4
2	C	46	LYS	2.4
1	B	29	GLY	2.4
1	B	63	LEU	2.3
1	A	291	HIS	2.3
1	B	60	VAL	2.3
1	B	31	VAL	2.2
2	D	81	GLU	2.2
1	B	379	SER	2.2
1	B	36	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	378	PHE	2.1
2	C	75	SER	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACT	A	407	4/4	0.76	0.28	70,70,70,71	0
3	ACT	A	409	4/4	0.87	0.26	67,68,68,68	0
3	ACT	A	408	4/4	0.89	0.20	86,86,87,88	0
4	ZN	B	407	1/1	0.96	0.04	45,45,45,45	0
4	ZN	A	410	1/1	0.96	0.05	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.