



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:15 AM GMT

PDB ID : 3JY6
Title : Crystal structure of LacI Transcriptional regulator from Lactobacillus brevis
Authors : Syed Ibrahim, B.; Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York
SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-09-21
Resolution : 1.97 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

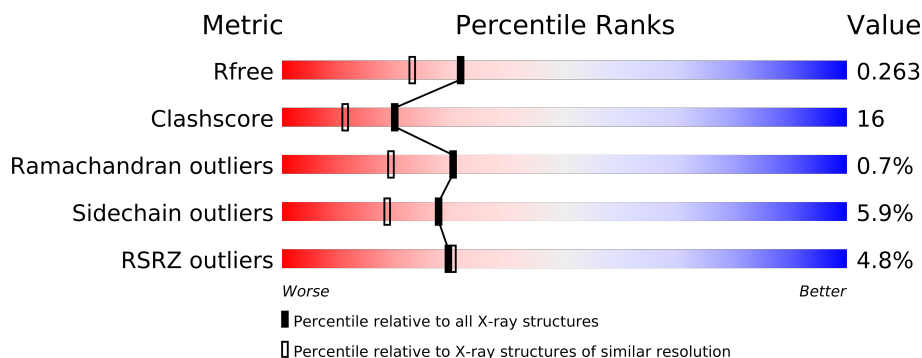
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.97 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	6577 (2.00-1.96)
Clashscore	79885	8091 (2.00-1.96)
Ramachandran outliers	78287	7989 (2.00-1.96)
Sidechain outliers	78261	7987 (2.00-1.96)
RSRZ outliers	66119	6578 (2.00-1.96)

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 ≥ 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	276	
1	B	276	
1	C	276	
1	D	276	

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	EDO	D	3318	-	X
3	EDO	D	3319	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8291 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 Transcriptional regulator, LacI family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2065	1307	353	398	7			
1	B	259	Total	C	N	O	S	0	0	0
			2027	1285	348	387	7			
1	C	254	Total	C	N	O	S	0	0	0
			1976	1256	337	376	7			
1	D	261	Total	C	N	O	S	0	0	0
			2038	1291	347	393	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	MET	-	EXPRESSION TAG	UNP Q03T70
A	62	SER	-	EXPRESSION TAG	UNP Q03T70
A	63	LEU	-	EXPRESSION TAG	UNP Q03T70
A	329	GLU	-	EXPRESSION TAG	UNP Q03T70
A	330	GLY	-	EXPRESSION TAG	UNP Q03T70
A	331	HIS	-	EXPRESSION TAG	UNP Q03T70
A	332	HIS	-	EXPRESSION TAG	UNP Q03T70
A	333	HIS	-	EXPRESSION TAG	UNP Q03T70
A	334	HIS	-	EXPRESSION TAG	UNP Q03T70
A	335	HIS	-	EXPRESSION TAG	UNP Q03T70
A	336	HIS	-	EXPRESSION TAG	UNP Q03T70
B	61	MET	-	EXPRESSION TAG	UNP Q03T70
B	62	SER	-	EXPRESSION TAG	UNP Q03T70
B	63	LEU	-	EXPRESSION TAG	UNP Q03T70
B	329	GLU	-	EXPRESSION TAG	UNP Q03T70
B	330	GLY	-	EXPRESSION TAG	UNP Q03T70
B	331	HIS	-	EXPRESSION TAG	UNP Q03T70
B	332	HIS	-	EXPRESSION TAG	UNP Q03T70
B	333	HIS	-	EXPRESSION TAG	UNP Q03T70
B	334	HIS	-	EXPRESSION TAG	UNP Q03T70
B	335	HIS	-	EXPRESSION TAG	UNP Q03T70

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	336	HIS	-	EXPRESSION TAG	UNP Q03T70
C	61	MET	-	EXPRESSION TAG	UNP Q03T70
C	62	SER	-	EXPRESSION TAG	UNP Q03T70
C	63	LEU	-	EXPRESSION TAG	UNP Q03T70
C	329	GLU	-	EXPRESSION TAG	UNP Q03T70
C	330	GLY	-	EXPRESSION TAG	UNP Q03T70
C	331	HIS	-	EXPRESSION TAG	UNP Q03T70
C	332	HIS	-	EXPRESSION TAG	UNP Q03T70
C	333	HIS	-	EXPRESSION TAG	UNP Q03T70
C	334	HIS	-	EXPRESSION TAG	UNP Q03T70
C	335	HIS	-	EXPRESSION TAG	UNP Q03T70
C	336	HIS	-	EXPRESSION TAG	UNP Q03T70
D	61	MET	-	EXPRESSION TAG	UNP Q03T70
D	62	SER	-	EXPRESSION TAG	UNP Q03T70
D	63	LEU	-	EXPRESSION TAG	UNP Q03T70
D	329	GLU	-	EXPRESSION TAG	UNP Q03T70
D	330	GLY	-	EXPRESSION TAG	UNP Q03T70
D	331	HIS	-	EXPRESSION TAG	UNP Q03T70
D	332	HIS	-	EXPRESSION TAG	UNP Q03T70
D	333	HIS	-	EXPRESSION TAG	UNP Q03T70
D	334	HIS	-	EXPRESSION TAG	UNP Q03T70
D	335	HIS	-	EXPRESSION TAG	UNP Q03T70
D	336	HIS	-	EXPRESSION TAG	UNP Q03T70

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is water.

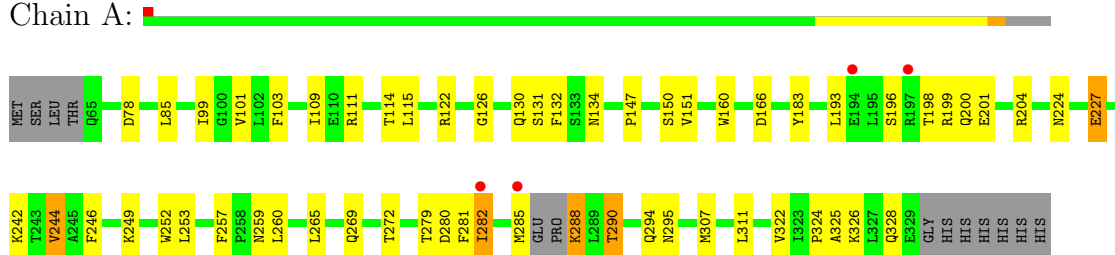
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	34	Total	O	0	0
			34	34		
4	C	50	Total	O	0	0
			50	50		
4	D	42	Total	O	0	0
			42	42		

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.

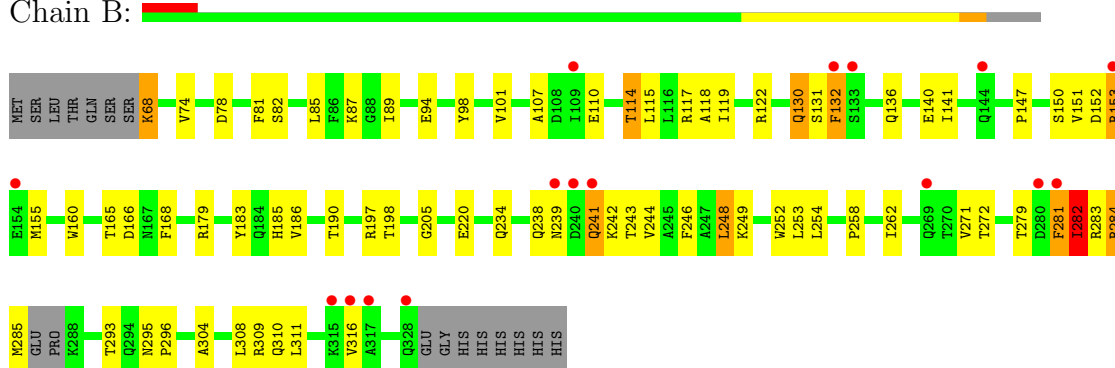
- Molecule 1: Transcriptional regulator, LacI family

Chain A:



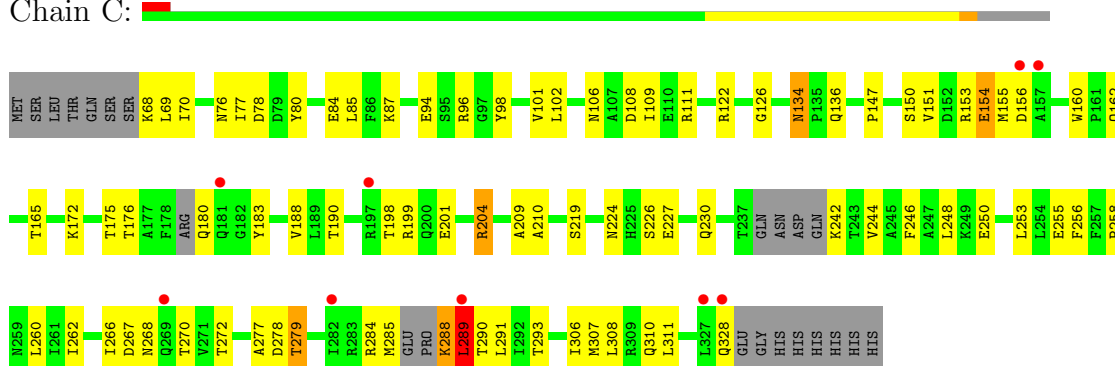
- Molecule 1: Transcriptional regulator, LacI family

Chain B:



- Molecule 1: Transcriptional regulator, LacI family

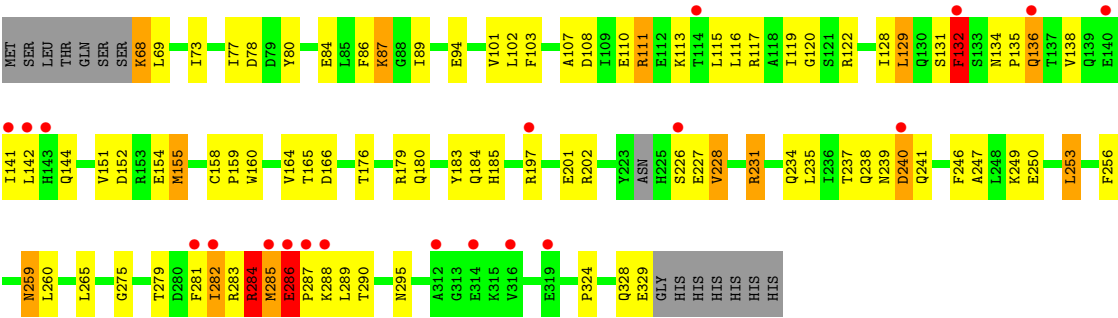
Chain C:



- Molecule 1: Transcriptional regulator, LacI family

Chain D:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.57Å 109.33Å 113.34Å 90.00° 95.17° 90.00°	Depositor
Resolution (Å)	40.41 – 1.97 40.40 – 1.97	Depositor EDS
% Data completeness (in resolution range)	88.3 (40.41-1.97) 88.5 (40.40-1.97)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.97Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.261 0.250 , 0.263	Depositor DCC
R_{free} test set	3111 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 65876 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8291	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: EDO, 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	0.47	1/2097 (0.0%)	0.74	4/2840 (0.1%)
1	B	0.43	0/2058	0.69	1/2788 (0.0%)
1	C	0.41	0/2005	0.69	2/2714 (0.1%)
1	D	0.55	1/2070 (0.0%)	0.90	8/2807 (0.3%)
All	All	0.47	2/8230 (0.0%)	0.76	15/11149 (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
1	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	286	GLU	CB-CG	-5.91	1.41	1.52
1	A	288	LYS	C-O	5.07	1.32	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	129	LEU	CA-CB-CG	9.30	136.68	115.30
1	D	129	LEU	CB-CG-CD2	-8.32	96.86	111.00
1	D	286	GLU	N-CA-C	-8.02	89.35	111.00
1	C	289	LEU	N-CA-C	7.75	131.93	111.00
1	D	132	PHE	N-CA-C	7.64	131.62	111.00
1	B	282	ILE	CB-CA-C	-7.17	97.27	111.60
1	D	286	GLU	CA-C-N	-7.09	97.25	117.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	286	GLU	N-CA-CB	6.33	121.99	110.60
1	A	288	LYS	CA-C-O	6.33	133.38	120.10
1	A	282	ILE	CB-CA-C	-6.24	99.12	111.60
1	D	284	ARG	N-CA-C	-6.06	94.65	111.00
1	C	154	GLU	N-CA-C	-5.48	96.19	111.00
1	A	288	LYS	N-CA-CB	5.18	119.93	110.60
1	A	288	LYS	N-CA-C	5.09	124.73	111.00
1	D	289	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	286	GLU	Mainchain

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	2065	0	2066	45	0
1	B	2027	0	2028	68	0
1	C	1976	0	1978	76	0
1	D	2038	0	2015	92	0
2	D	1	0	0	0	0
3	D	8	0	12	16	0
4	A	50	0	0	5	0
4	B	34	0	0	5	0
4	C	50	0	0	9	0
4	D	42	0	0	6	0
All	All	8291	0	8099	259	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 16.

All (259) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:126:GLY:HA3	1:A:307:MET:HE1	1.28	1.13
1:C:154:GLU:OE1	1:C:201:GLU:HG3	1.51	1.09
1:A:134:ASN:HB2	4:A:355:HOH:O	1.64	0.97
1:C:68:LYS:HD3	4:C:379:HOH:O	1.65	0.97
1:D:107:ALA:HA	1:D:132:PHE:HZ	1.33	0.92
1:C:126:GLY:HA3	1:C:307:MET:HE1	1.51	0.91
1:C:134:ASN:HD21	1:C:136:GLN:HB2	1.32	0.91
1:D:107:ALA:HA	1:D:132:PHE:CZ	2.05	0.90
1:B:283:ARG:HH22	1:B:293:THR:CG2	1.93	0.81
1:B:185:HIS:HB2	1:B:241:GLN:HG3	1.62	0.81
3:D:3318:EDO:H12	4:D:4:HOH:O	1.80	0.80
1:C:94:GLU:OE2	1:D:111:ARG:HD2	1.83	0.79
1:B:283:ARG:NH2	1:B:293:THR:CG2	2.47	0.78
1:D:134:ASN:HD21	1:D:136:GLN:HG3	1.48	0.78
1:C:224:ASN:HD22	1:C:227:GLU:H	1.31	0.77
1:A:122:ARG:HH21	1:B:68:LYS:N	1.84	0.76
1:D:154:GLU:HG3	1:D:164:VAL:HG11	1.68	0.76
1:D:279:THR:HB	1:D:282:ILE:CB	2.15	0.75
1:A:224:ASN:HB3	1:A:227:GLU:HB3	1.70	0.74
1:C:109:ILE:HD11	4:C:346:HOH:O	1.87	0.74
1:C:255:GLU:HG3	1:D:284:ARG:HH12	1.54	0.73
3:D:3318:EDO:H21	3:D:3319:EDO:H22	1.71	0.72
3:D:3318:EDO:H21	3:D:3319:EDO:C2	2.19	0.72
1:D:239:ASN:ND2	1:D:240:ASP:H	1.88	0.72
1:B:74:VAL:HA	1:B:130:GLN:HG3	1.70	0.72
1:C:328:GLN:HB3	4:C:380:HOH:O	1.90	0.71
1:C:183:TYR:HB3	1:C:244:VAL:HG22	1.72	0.71
1:D:135:PRO:HG3	1:D:155:MET:HE2	1.73	0.71
1:D:283:ARG:O	1:D:284:ARG:HG3	1.90	0.71
1:D:227:GLU:HB3	1:D:231:ARG:HH12	1.55	0.71
1:A:279:THR:HG21	1:A:281:PHE:CZ	2.25	0.70
1:A:78:ASP:OD2	1:B:87:LYS:HE3	1.91	0.70
1:B:85:LEU:HD11	1:B:151:VAL:HG11	1.74	0.69
1:C:76:ASN:OD1	1:C:78:ASP:HB2	1.92	0.69
1:C:94:GLU:HG3	1:D:111:ARG:NH1	2.06	0.69
1:D:281:PHE:C	1:D:281:PHE:CD1	2.65	0.69
1:B:279:THR:HG21	1:B:281:PHE:CE2	2.29	0.68
1:A:279:THR:HG21	1:A:281:PHE:CE2	2.29	0.68
1:A:249:LYS:HG2	4:A:24:HOH:O	1.92	0.68
1:C:85:LEU:HD11	1:C:151:VAL:HG11	1.76	0.67
1:A:285:MET:HE1	1:B:262:ILE:HD11	1.76	0.67
1:B:185:HIS:CB	1:B:241:GLN:HG3	2.24	0.66
1:D:134:ASN:HD21	1:D:136:GLN:CG	2.08	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:199:ARG:HG2	4:C:347:HOH:O	1.96	0.66
1:C:80:TYR:CZ	1:C:84:GLU:HG3	2.31	0.65
1:C:102:LEU:HD23	1:D:102:LEU:HD23	1.79	0.65
1:C:183:TYR:HB3	1:C:244:VAL:CG2	2.27	0.65
1:D:250:GLU:H	3:D:3318:EDO:C2	2.09	0.65
1:C:262:ILE:HD12	1:D:285:MET:HG2	1.78	0.65
1:A:183:TYR:HB3	1:A:244:VAL:HG22	1.78	0.65
1:B:253:LEU:CD2	1:B:282:ILE:HG21	2.27	0.64
1:D:249:LYS:HG2	3:D:3318:EDO:H22	1.80	0.64
1:C:224:ASN:ND2	1:C:227:GLU:H	1.96	0.64
3:D:3318:EDO:H21	3:D:3319:EDO:O2	1.97	0.64
1:A:259:ASN:HD21	1:B:285:MET:HA	1.63	0.64
1:A:126:GLY:CA	1:A:307:MET:HE1	2.18	0.63
1:C:224:ASN:ND2	1:C:227:GLU:HG3	2.13	0.63
1:D:120:GLY:HA3	1:D:142:LEU:O	1.98	0.63
1:B:279:THR:HG22	1:B:281:PHE:H	1.63	0.63
1:C:126:GLY:CA	1:C:307:MET:HE1	2.26	0.63
1:C:70:ILE:HD12	1:C:307:MET:HE2	1.81	0.62
1:A:259:ASN:ND2	1:B:285:MET:HA	2.14	0.62
1:C:126:GLY:HA3	1:C:307:MET:CE	2.27	0.62
1:A:198:THR:HG23	4:A:343:HOH:O	2.00	0.62
1:D:197:ARG:O	1:D:201:GLU:HG3	1.99	0.62
1:C:76:ASN:HD21	1:D:87:LYS:NZ	1.97	0.61
1:D:68:LYS:NZ	1:D:68:LYS:HB3	2.14	0.61
1:D:249:LYS:HA	3:D:3318:EDO:H22	1.83	0.61
1:A:99:ILE:HD12	1:B:122:ARG:HH12	1.66	0.61
1:D:281:PHE:O	1:D:283:ARG:N	2.34	0.60
1:C:262:ILE:CD1	1:D:285:MET:HG2	2.31	0.60
1:C:165:THR:HG23	4:C:342:HOH:O	2.01	0.60
1:D:176:THR:O	1:D:180:GLN:HG3	2.02	0.60
1:B:253:LEU:HD21	1:B:282:ILE:HG21	1.84	0.59
1:B:283:ARG:NH2	1:B:293:THR:HG21	2.18	0.59
1:A:279:THR:CG2	1:A:281:PHE:CE2	2.85	0.59
1:A:242:LYS:HE3	1:A:269:GLN:O	2.04	0.58
1:C:96:ARG:HG3	1:C:308:LEU:HD13	1.85	0.58
1:C:190:THR:HB	1:C:248:LEU:HD22	1.85	0.58
1:D:249:LYS:HG2	3:D:3318:EDO:C1	2.33	0.58
1:A:101:VAL:HG13	1:B:101:VAL:HG13	1.85	0.58
1:C:154:GLU:OE1	1:C:201:GLU:CG	2.39	0.58
1:D:253:LEU:HD11	1:D:275:GLY:HA3	1.84	0.58
1:A:285:MET:HE3	1:B:258:PRO:HB3	1.85	0.57
1:D:288:LYS:HA	4:D:355:HOH:O	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:250:GLU:OE2	1:C:277:ALA:HB1	2.04	0.56
1:A:244:VAL:HG13	1:A:272:THR:HG23	1.86	0.56
1:B:110:GLU:O	1:B:114:THR:HG22	2.04	0.56
1:D:202:ARG:HH12	3:D:3319:EDO:H21	1.69	0.56
1:D:249:LYS:HG2	3:D:3318:EDO:H12	1.87	0.56
1:B:190:THR:HB	1:B:248:LEU:HD22	1.88	0.56
1:D:283:ARG:C	1:D:284:ARG:HG3	2.25	0.55
1:B:136:GLN:O	1:B:140:GLU:HG3	2.06	0.55
1:B:197:ARG:CB	4:B:351:HOH:O	2.54	0.55
1:C:153:ARG:HB2	4:C:343:HOH:O	2.07	0.55
1:D:290:THR:CG2	1:D:329:GLU:HG3	2.37	0.55
1:B:283:ARG:NH2	1:B:293:THR:HG22	2.21	0.55
1:B:131:SER:O	1:B:153:ARG:HG2	2.07	0.54
1:C:198:THR:HG23	4:C:353:HOH:O	2.05	0.54
1:D:281:PHE:C	1:D:283:ARG:H	2.11	0.54
1:C:328:GLN:HG2	4:C:380:HOH:O	2.07	0.54
1:D:113:LYS:NZ	1:D:141:ILE:HD11	2.21	0.54
1:B:283:ARG:NH1	4:B:352:HOH:O	2.39	0.54
1:D:231:ARG:HD2	4:D:360:HOH:O	2.07	0.54
1:D:239:ASN:OD1	1:D:241:GLN:HB2	2.08	0.54
1:D:227:GLU:CD	1:D:227:GLU:H	2.11	0.54
1:A:253:LEU:HG	1:A:257:PHE:CD2	2.43	0.54
1:A:166:ASP:OD1	1:A:324:PRO:HA	2.08	0.53
1:C:188:VAL:HG13	1:C:248:LEU:HD13	1.89	0.53
1:D:281:PHE:C	1:D:283:ARG:N	2.62	0.53
1:C:328:GLN:HG3	1:C:328:GLN:O	2.09	0.52
1:C:154:GLU:HG3	1:C:198:THR:HG22	1.90	0.52
1:C:284:ARG:NH1	1:C:284:ARG:HB3	2.25	0.52
1:B:81:PHE:CD1	1:B:296:PRO:HB3	2.44	0.52
1:B:115:LEU:O	1:B:119:ILE:HD13	2.08	0.52
1:C:154:GLU:CG	1:C:198:THR:HG22	2.40	0.52
1:C:101:VAL:CG1	1:D:101:VAL:HG13	2.40	0.52
1:B:281:PHE:CD1	1:B:281:PHE:C	2.84	0.51
1:C:108:ASP:HB3	1:C:111:ARG:HB3	1.91	0.51
1:D:279:THR:HG22	1:D:282:ILE:H	1.76	0.51
1:C:253:LEU:O	1:C:258:PRO:HD3	2.10	0.51
1:C:68:LYS:HB3	1:C:98:TYR:CD1	2.46	0.51
1:D:111:ARG:O	1:D:115:LEU:HG	2.11	0.51
1:C:85:LEU:CD1	1:C:151:VAL:HG11	2.41	0.51
1:D:286:GLU:C	1:D:288:LYS:H	2.13	0.51
1:B:279:THR:HG21	1:B:281:PHE:CD2	2.46	0.51
1:B:85:LEU:O	1:B:89:ILE:HD12	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:109:ILE:HD13	1:A:132:PHE:HB2	1.94	0.50
1:C:256:PHE:O	1:C:260:LEU:HD13	2.10	0.50
1:B:238:GLN:HG3	1:B:239:ASN:N	2.26	0.50
1:B:150:SER:HB3	1:B:160:TRP:HE1	1.76	0.50
1:B:118:ALA:HB1	1:B:122:ARG:HH11	1.76	0.50
1:D:249:LYS:HG2	3:D:3318:EDO:C2	2.41	0.50
1:D:290:THR:HG21	1:D:329:GLU:HG3	1.94	0.50
1:D:108:ASP:OD1	1:D:110:GLU:HB2	2.11	0.50
1:B:239:ASN:CB	1:B:241:GLN:NE2	2.75	0.49
1:D:103:PHE:HB3	1:D:115:LEU:HD13	1.94	0.49
1:B:183:TYR:CD1	1:B:242:LYS:HG2	2.47	0.49
1:D:151:VAL:HG12	1:D:152:ASP:N	2.27	0.49
1:C:176:THR:O	1:C:180:GLN:HG3	2.12	0.49
1:C:224:ASN:HD22	1:C:227:GLU:N	2.04	0.49
1:D:185:HIS:HE1	1:D:235:LEU:O	1.96	0.49
1:B:197:ARG:HB2	4:B:351:HOH:O	2.12	0.49
1:B:165:THR:HG22	1:B:166:ASP:N	2.27	0.49
1:C:155:MET:CB	1:C:162:GLN:HE22	2.26	0.48
1:A:244:VAL:HG13	1:A:272:THR:CG2	2.44	0.48
1:C:277:ALA:HB3	1:C:291:LEU:HD22	1.95	0.48
1:A:259:ASN:ND2	1:B:284:ARG:O	2.44	0.48
1:D:260:LEU:HD22	1:D:265:LEU:HD23	1.96	0.48
1:C:267:ASP:O	1:C:268:ASN:HB2	2.14	0.48
1:B:117:ARG:HG2	1:B:141:ILE:HG23	1.95	0.47
1:B:239:ASN:CB	1:B:241:GLN:CD	2.83	0.47
1:B:279:THR:CG2	1:B:281:PHE:CD2	2.98	0.47
1:D:113:LYS:O	1:D:117:ARG:HG3	2.14	0.47
1:A:85:LEU:HD22	1:A:130:GLN:HG3	1.96	0.47
1:B:249:LYS:HG2	4:B:337:HOH:O	2.13	0.47
1:C:87:LYS:HG3	1:D:77:ILE:HD11	1.95	0.47
1:A:294:GLN:O	1:A:295:ASN:HB2	2.15	0.47
1:D:239:ASN:ND2	1:D:240:ASP:N	2.60	0.47
1:D:290:THR:HB	1:D:329:GLU:HG3	1.97	0.47
1:B:220:GLU:HG2	1:B:252:TRP:HZ2	1.79	0.47
1:D:250:GLU:H	3:D:3318:EDO:H22	1.78	0.46
1:C:77:ILE:HD13	1:D:86:PHE:HD2	1.81	0.46
1:D:80:TYR:CZ	1:D:84:GLU:HG3	2.51	0.46
1:D:247:ALA:HB3	1:D:253:LEU:CD1	2.46	0.46
1:A:260:LEU:HG	1:A:265:LEU:HD23	1.97	0.46
1:D:249:LYS:CG	3:D:3318:EDO:H22	2.45	0.46
1:B:152:ASP:O	1:B:198:THR:HG21	2.16	0.46
1:C:201:GLU:OE1	1:C:204:ARG:NH1	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:328:GLN:CG	4:C:380:HOH:O	2.62	0.45
1:B:238:GLN:HG3	1:B:239:ASN:H	1.81	0.45
1:C:111:ARG:NH1	1:D:94:GLU:HG3	2.32	0.45
1:A:111:ARG:NH1	1:B:94:GLU:HG3	2.31	0.45
1:C:172:LYS:HG3	1:C:209:ALA:HB2	1.98	0.45
3:D:3318:EDO:C2	3:D:3319:EDO:H22	2.43	0.45
1:B:82:SER:OG	1:B:130:GLN:NE2	2.49	0.45
1:B:183:TYR:N	1:B:242:LYS:HZ2	2.14	0.45
1:D:165:THR:HG22	1:D:166:ASP:N	2.32	0.45
1:D:227:GLU:O	1:D:228:VAL:CB	2.64	0.45
1:B:168:PHE:CE1	1:B:205:GLY:HA2	2.52	0.45
1:A:322:VAL:HG12	4:A:10:HOH:O	2.16	0.45
1:C:226:SER:O	1:C:230:GLN:HG3	2.17	0.45
1:D:166:ASP:OD1	1:D:324:PRO:HA	2.16	0.45
1:C:69:LEU:HD11	1:D:122:ARG:HD3	1.98	0.45
1:D:227:GLU:O	1:D:228:VAL:HG23	2.17	0.44
1:D:159:PRO:HG2	1:D:160:TRP:CE3	2.52	0.44
1:C:101:VAL:HG13	1:D:101:VAL:HG13	1.99	0.44
1:A:147:PRO:HG2	1:A:307:MET:HE3	1.98	0.44
1:C:106:ASN:OD1	1:D:87:LYS:NZ	2.50	0.44
1:C:242:LYS:HA	1:C:270:THR:O	2.18	0.44
1:C:278:ASP:OD1	1:C:293:THR:HB	2.17	0.44
1:D:110:GLU:OE1	1:D:113:LYS:HD2	2.18	0.44
1:D:68:LYS:HZ3	1:D:68:LYS:HB3	1.81	0.44
1:B:304:ALA:O	1:B:308:LEU:HG	2.18	0.44
1:A:307:MET:HE2	1:A:311:LEU:HD11	1.99	0.44
1:D:250:GLU:CB	3:D:3318:EDO:O2	2.65	0.44
1:C:289:LEU:O	1:C:290:THR:HB	2.16	0.44
1:D:281:PHE:CD1	1:D:282:ILE:N	2.86	0.44
1:C:150:SER:HB2	1:C:160:TRP:HE1	1.83	0.44
1:A:103:PHE:HB3	1:A:115:LEU:HD13	2.00	0.43
1:C:307:MET:HE3	1:C:311:LEU:HG	2.00	0.43
1:B:107:ALA:HA	1:B:132:PHE:CZ	2.53	0.43
1:C:134:ASN:ND2	1:C:136:GLN:HB2	2.15	0.43
1:C:224:ASN:HD22	1:C:227:GLU:HG3	1.84	0.43
1:B:147:PRO:HB3	1:B:310:GLN:HB3	2.00	0.43
1:A:183:TYR:CB	1:A:244:VAL:HG22	2.48	0.43
1:D:328:GLN:NE2	4:D:354:HOH:O	2.44	0.43
1:B:185:HIS:CG	1:B:241:GLN:HG3	2.54	0.42
1:B:130:GLN:HG3	1:B:130:GLN:O	2.19	0.42
1:A:328:GLN:HG3	1:A:328:GLN:O	2.19	0.42
1:D:227:GLU:O	1:D:228:VAL:HB	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:259:ASN:HA	1:D:259:ASN:HD22	1.64	0.42
1:B:220:GLU:HG2	1:B:252:TRP:CZ2	2.54	0.42
1:C:175:THR:CG2	1:C:210:ALA:HB2	2.49	0.42
1:C:266:ILE:HG23	1:C:272:THR:HA	2.01	0.42
1:A:193:LEU:O	1:A:200:GLN:HG3	2.20	0.42
1:A:325:ALA:O	1:A:326:LYS:HD3	2.20	0.42
1:B:186:VAL:HG22	1:B:244:VAL:CG1	2.50	0.42
1:D:116:LEU:HD22	1:D:142:LEU:HD13	2.01	0.42
1:C:147:PRO:HG2	1:C:307:MET:CE	2.50	0.42
1:B:241:GLN:HB3	1:B:241:GLN:HE21	1.51	0.42
1:A:285:MET:CE	1:B:258:PRO:HB3	2.50	0.42
1:A:201:GLU:OE2	1:A:204:ARG:NH1	2.53	0.42
1:D:179:ARG:HA	1:D:183:TYR:O	2.20	0.42
1:A:196:SER:HB3	1:A:199:ARG:CD	2.50	0.42
1:D:281:PHE:C	1:D:281:PHE:HD1	2.22	0.41
1:B:244:VAL:HG23	1:B:272:THR:HG23	2.01	0.41
1:C:288:LYS:HG2	1:C:288:LYS:O	2.20	0.41
1:D:250:GLU:HB2	3:D:3318:EDO:O2	2.19	0.41
1:C:250:GLU:OE2	1:C:279:THR:HB	2.20	0.41
1:A:85:LEU:HD11	1:A:151:VAL:HG11	2.03	0.41
1:A:150:SER:HB2	1:A:160:TRP:HE1	1.85	0.41
1:B:254:LEU:HD21	1:B:282:ILE:HD13	2.01	0.41
1:C:87:LYS:HE3	1:D:78:ASP:OD2	2.19	0.41
1:C:122:ARG:HE	1:D:69:LEU:HD12	1.85	0.41
1:A:280:ASP:HB2	4:A:338:HOH:O	2.20	0.41
1:B:68:LYS:HB2	1:B:98:TYR:CD1	2.54	0.41
1:C:306:ILE:O	1:C:310:GLN:HG3	2.21	0.41
1:B:197:ARG:HB3	4:B:351:HOH:O	2.17	0.41
1:D:111:ARG:NH2	4:D:345:HOH:O	2.54	0.41
1:B:243:THR:HG22	1:B:244:VAL:N	2.36	0.41
1:D:113:LYS:HZ2	1:D:141:ILE:HD11	1.85	0.41
1:A:290:THR:O	1:A:290:THR:HG22	2.21	0.41
1:B:130:GLN:CG	1:B:130:GLN:O	2.69	0.41
1:D:231:ARG:CD	4:D:360:HOH:O	2.68	0.41
1:C:77:ILE:HG22	1:C:102:LEU:HD21	2.03	0.41
1:D:73:ILE:HD11	1:D:119:ILE:HD12	2.03	0.41
1:D:89:ILE:CD1	1:D:128:ILE:HG21	2.51	0.41
1:D:290:THR:HG21	1:D:329:GLU:CG	2.50	0.41
1:D:290:THR:CB	1:D:329:GLU:HA	2.51	0.41
1:C:284:ARG:HG3	1:C:284:ARG:O	2.21	0.41
1:D:234:GLN:O	1:D:238:GLN:N	2.53	0.41
1:B:183:TYR:CG	1:B:242:LYS:NZ	2.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:290:THR:HB	1:D:329:GLU:HA	2.02	0.40
1:D:256:PHE:O	1:D:260:LEU:HG	2.21	0.40
1:A:252:TRP:HA	1:A:252:TRP:CE3	2.57	0.40
1:B:309:ARG:NH1	1:B:316:VAL:HG13	2.37	0.40
1:D:138:VAL:O	1:D:142:LEU:HB2	2.22	0.40
1:B:243:THR:O	1:B:271:VAL:HA	2.22	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	259/276 (94%)	252 (97%)	7 (3%)	0	100	100
1	B	255/276 (92%)	247 (97%)	8 (3%)	0	100	100
1	C	246/276 (89%)	233 (95%)	13 (5%)	0	100	100
1	D	257/276 (93%)	242 (94%)	8 (3%)	7 (3%)	8	2
All	All	1017/1104 (92%)	974 (96%)	36 (4%)	7 (1%)	30	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	131	SER
1	D	228	VAL
1	D	282	ILE
1	D	287	PRO
1	D	132	PHE
1	D	284	ARG
1	D	285	MET

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	226/240 (94%)	218 (96%)	8 (4%)	48	41
1	B	219/240 (91%)	202 (92%)	17 (8%)	18	10
1	C	213/240 (89%)	204 (96%)	9 (4%)	40	32
1	D	219/240 (91%)	201 (92%)	18 (8%)	17	9
All	All	877/960 (91%)	825 (94%)	52 (6%)	28	18

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	131	SER
1	A	227	GLU
1	A	244	VAL
1	A	246	PHE
1	A	282	ILE
1	A	288	LYS
1	A	290	THR
1	B	68	LYS
1	B	78	ASP
1	B	114	THR
1	B	130	GLN
1	B	132	PHE
1	B	153	ARG
1	B	155	MET
1	B	179	ARG
1	B	234	GLN
1	B	241	GLN
1	B	246	PHE
1	B	248	LEU
1	B	281	PHE
1	B	282	ILE
1	B	284	ARG
1	B	295	ASN
1	B	311	LEU
1	C	134	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	156	ASP
1	C	204	ARG
1	C	219	SER
1	C	246	PHE
1	C	279	THR
1	C	285	MET
1	C	288	LYS
1	C	289	LEU
1	D	68	LYS
1	D	87	LYS
1	D	111	ARG
1	D	129	LEU
1	D	132	PHE
1	D	136	GLN
1	D	144	GLN
1	D	155	MET
1	D	158	CYS
1	D	184	GLN
1	D	226	SER
1	D	231	ARG
1	D	237	THR
1	D	240	ASP
1	D	246	PHE
1	D	253	LEU
1	D	259	ASN
1	D	295	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	224	ASN
1	A	230	GLN
1	A	234	GLN
1	A	259	ASN
1	A	295	ASN
1	B	130	GLN
1	B	145	GLN
1	B	162	GLN
1	B	184	GLN
1	B	295	ASN
1	B	328	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	76	ASN
1	C	134	ASN
1	C	162	GLN
1	C	224	ASN
1	C	230	GLN
1	C	259	ASN
1	D	134	ASN
1	D	184	GLN
1	D	239	ASN
1	D	241	GLN
1	D	259	ASN
1	D	295	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	EDO	D	3318	-	3,3,3	0.79	0	2,2,2	0.41	0
3	EDO	D	3319	-	3,3,3	0.46	0	2,2,2	1.30	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	EDO	D	3318	-	-	0/1/1/1	0/0/0/0
3	EDO	D	3319	-	-	0/1/1/1	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, 95th 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 ²)	Q<0.9
1	A	263/276 (95%)	0.32	4 (1%) 70 73	11, 24, 40, 47	1 (0%)
1	B	259/276 (93%)	0.60	16 (6%) 20 21	11, 28, 46, 51	3 (1%)
1	C	254/276 (92%)	0.54	9 (3%) 42 43	11, 29, 44, 52	1 (0%)
1	D	261/276 (94%)	0.61	20 (7%) 13 13	10, 28, 47, 58	3 (1%)
All	All	1037/1104 (93%)	0.52	49 (4%) 29 31	10, 28, 45, 58	8 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	SER	5.3
1	C	289	LEU	4.7
1	B	240	ASP	4.7
1	B	281	PHE	4.6
1	D	143	HIS	4.5
1	B	132	PHE	4.0
1	C	327	LEU	3.7
1	D	312	ALA	3.5
1	D	281	PHE	3.1
1	D	282	ILE	3.1
1	B	239	ASN	3.1
1	D	197	ARG	3.0
1	B	144	GLN	3.0
1	D	142	LEU	3.0
1	D	136	GLN	2.9
1	D	286	GLU	2.8
1	B	315	LYS	2.8
1	A	282	ILE	2.7
1	A	197	ARG	2.7
1	D	288	LYS	2.7
1	C	282	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	157	ALA	2.6
1	C	181	GLN	2.6
1	A	285	MET	2.6
1	D	132	PHE	2.6
1	C	269	GLN	2.6
1	B	153	ARG	2.5
1	C	328	GLN	2.5
1	D	287	PRO	2.5
1	B	154	GLU	2.5
1	D	114	THR	2.5
1	D	226	SER	2.4
1	C	156	ASP	2.4
1	D	240	ASP	2.4
1	B	109	ILE	2.4
1	A	194	GLU	2.3
1	D	141	ILE	2.3
1	B	241	GLN	2.2
1	B	269	GLN	2.2
1	B	280	ASP	2.2
1	D	140	GLU	2.2
1	C	197	ARG	2.2
1	D	314	GLU	2.2
1	B	328	GLN	2.2
1	B	316	VAL	2.2
1	D	285	MET	2.1
1	B	317	ALA	2.1
1	D	319	GLU	2.1
1	D	316	VAL	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, 95th 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 ²)	Q<0.9
3	EDO	D	3318	4/4	0.50	15.33	31,31,32,33	0
3	EDO	D	3319	4/4	0.26	5.75	38,39,40,40	0
2	CL	D	1	1/1	0.10	-0.17	27,27,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.