



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:58 PM UTC

PDB ID : 9HUD / pdb_00009hud
Title : Alpha-1-antitrypsin in the cleaved conformation in complex with a conformationally nonselective Fab fragment
Authors : Irving, J.A.; Aldobiyan, I.F.
Deposited on : 2024-12-22
Resolution : 2.42 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

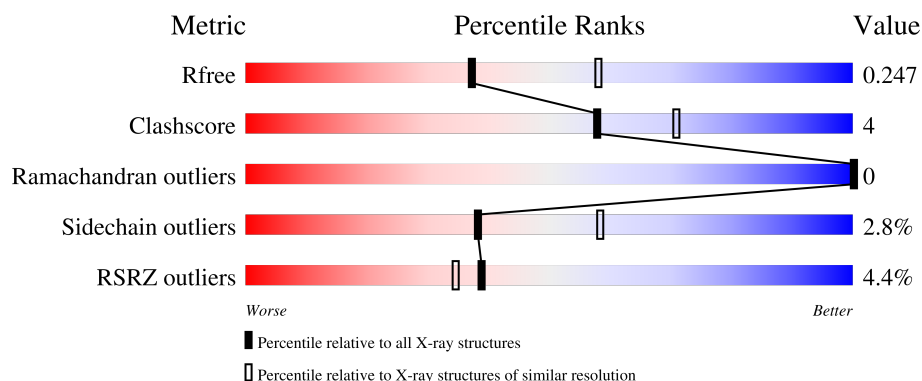
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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.



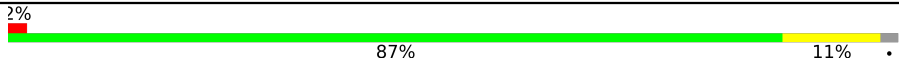
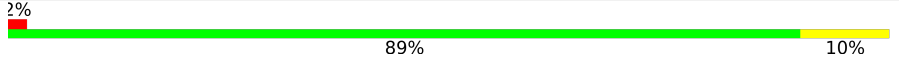
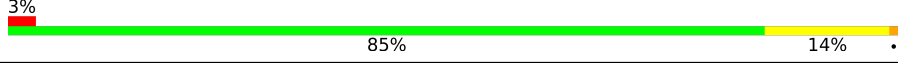
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	364	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>9%</div> </div> </div>
1	C	364	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>9%</div> </div> </div>
2	B	40	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>15%</div> <div>20%</div> </div> </div>
2	D	40	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>22%</div> <div>18%</div> </div> </div>
3	H	218	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	I	218	
4	L	214	
4	M	214	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GLY	H	301	-	X	-	-
6	GLY	H	302	-	X	-	-
6	GLY	I	301	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 12718 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 Alpha-1-antitrypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	2	0
			2516	1620	404	486	6			
1	C	332	Total	C	N	O	S	0	1	0
			2533	1630	403	493	7			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP P01009
A	-8	ARG	-	expression tag	UNP P01009
A	-7	GLY	-	expression tag	UNP P01009
A	-6	SER	-	expression tag	UNP P01009
A	-5	HIS	-	expression tag	UNP P01009
A	-4	HIS	-	expression tag	UNP P01009
A	-3	HIS	-	expression tag	UNP P01009
A	-2	HIS	-	expression tag	UNP P01009
A	-1	HIS	-	expression tag	UNP P01009
A	0	HIS	-	expression tag	UNP P01009
A	1	THR	-	expression tag	UNP P01009
C	-9	MET	-	initiating methionine	UNP P01009
C	-8	ARG	-	expression tag	UNP P01009
C	-7	GLY	-	expression tag	UNP P01009
C	-6	SER	-	expression tag	UNP P01009
C	-5	HIS	-	expression tag	UNP P01009
C	-4	HIS	-	expression tag	UNP P01009
C	-3	HIS	-	expression tag	UNP P01009
C	-2	HIS	-	expression tag	UNP P01009
C	-1	HIS	-	expression tag	UNP P01009
C	0	HIS	-	expression tag	UNP P01009
C	1	THR	-	expression tag	UNP P01009

- Molecule 2 is a protein called Short peptide from AAT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	32	Total	C	N	O	S	0	0	0
			244	164	38	40	2			
2	D	33	Total	C	N	O	S	0	0	0
			255	168	40	45	2			

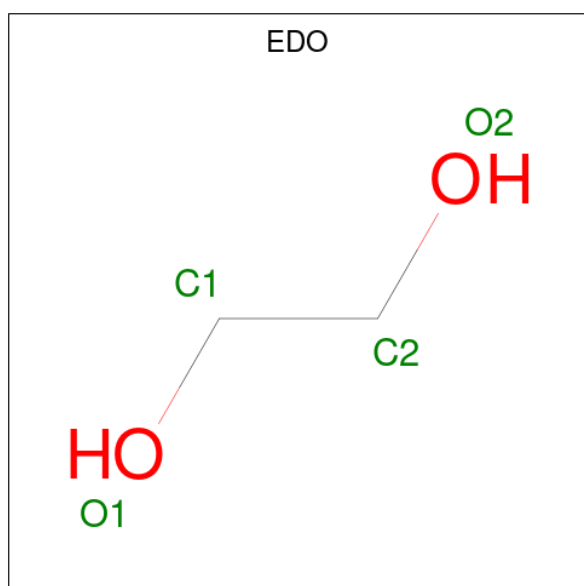
- Molecule 3 is a protein called FAB 9C5 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	217	Total	C	N	O	S	0	3	0
			1613	1017	268	321	7			
3	I	214	Total	C	N	O	S	0	3	0
			1612	1016	266	323	7			

- Molecule 4 is a protein called FAB 9C5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total	C	N	O	S	0	1	0
			1646	1030	277	333	6			
4	M	213	Total	C	N	O	S	0	1	0
			1643	1031	277	329	6			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



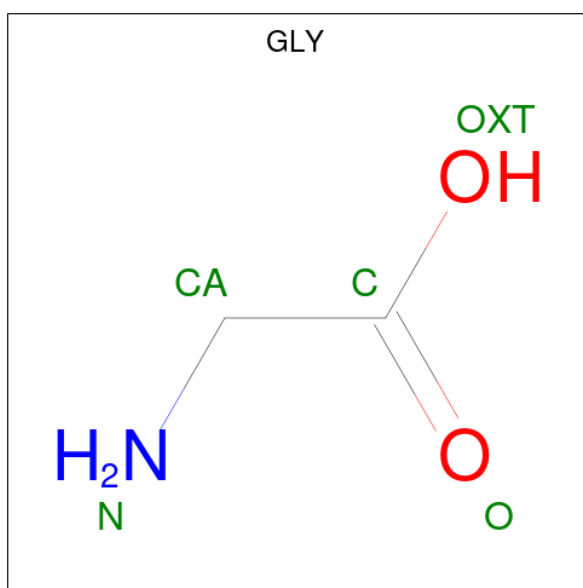
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	N	O	0	0
			5	2	1	2		
6	H	1	Total	C	N	O	0	0
			5	2	1	2		
6	I	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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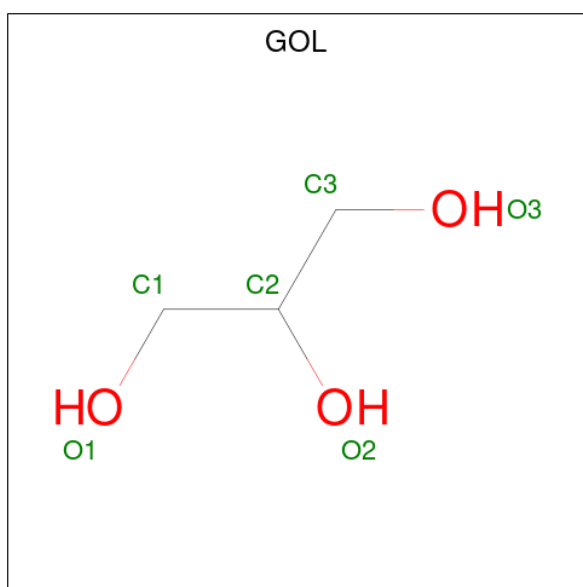
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Cl	0	0
			1	1		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

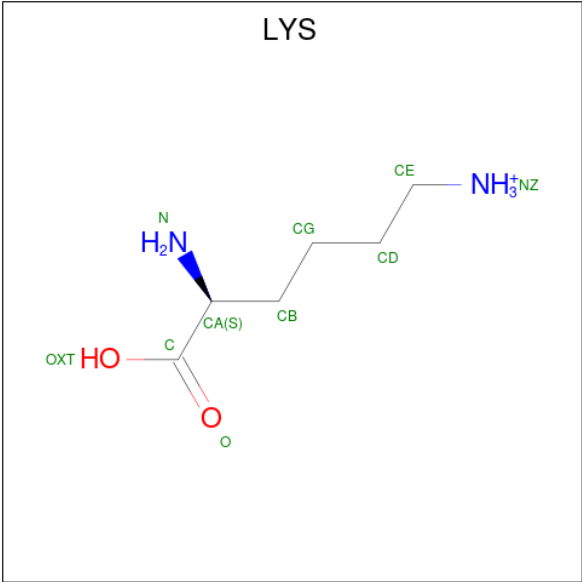
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	1	Total	Na	0	0
			1	1		
8	M	1	Total	Na	0	0
			1	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	N	O	0	0
			10	6	2	2		

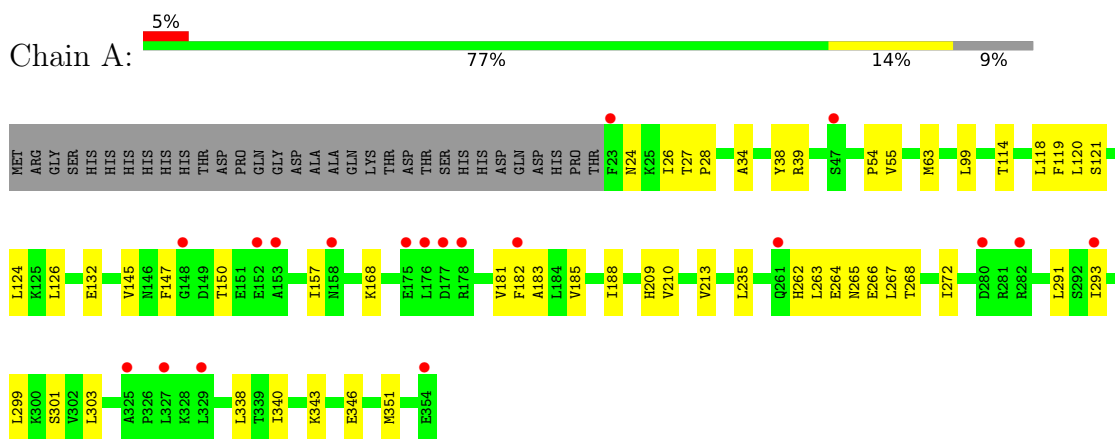
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	66	Total	O	0	0
			66	66		
11	B	8	Total	O	0	0
			8	8		
11	C	81	Total	O	0	0
			81	81		
11	D	6	Total	O	0	0
			6	6		
11	H	102	Total	O	0	0
			102	102		
11	L	102	Total	O	0	1
			103	103		
11	I	121	Total	O	0	0
			121	121		
11	M	110	Total	O	0	0
			110	110		

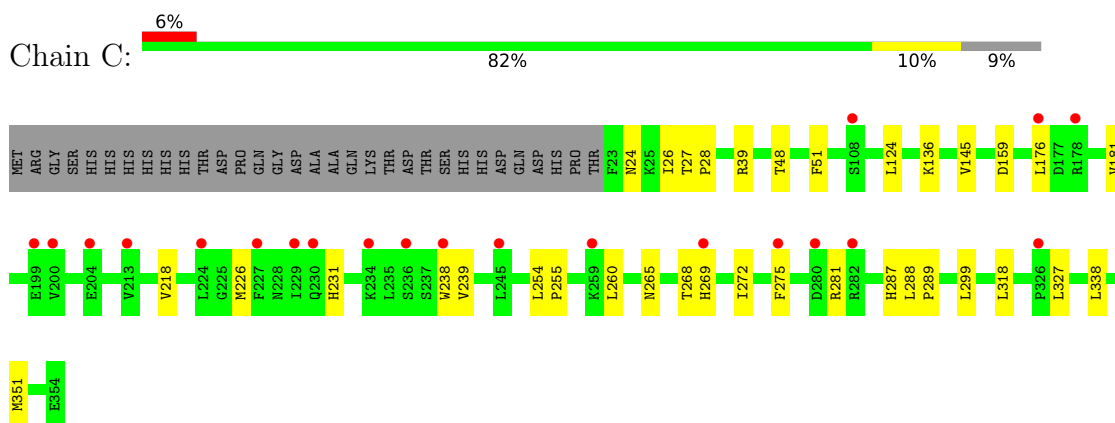
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

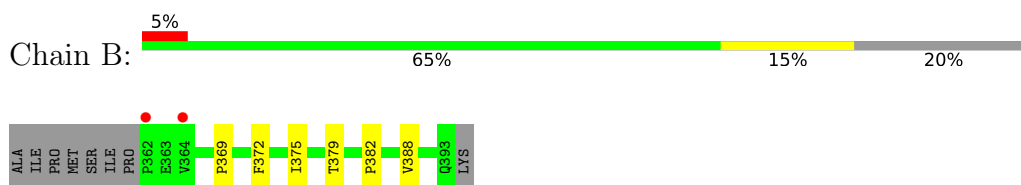
- Molecule 1: Alpha-1-antitrypsin



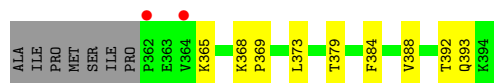
- Molecule 1: Alpha-1-antitrypsin



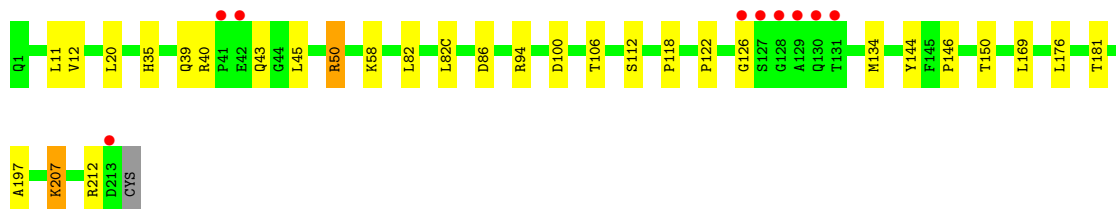
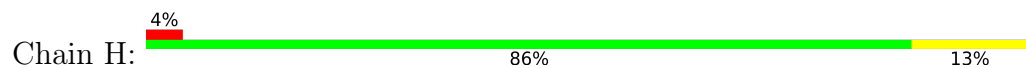
- Molecule 2: Short peptide from AAT



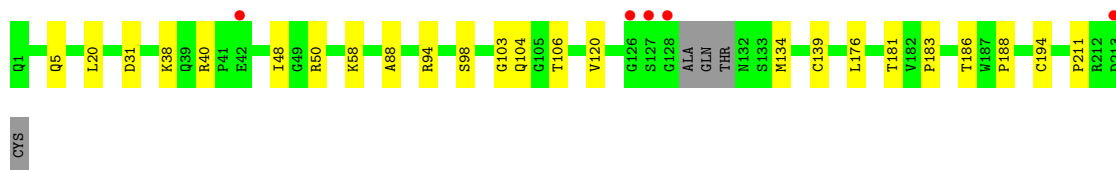
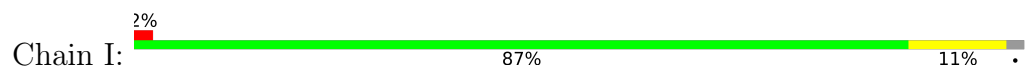
- Molecule 2: Short peptide from AAT



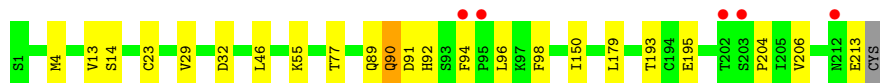
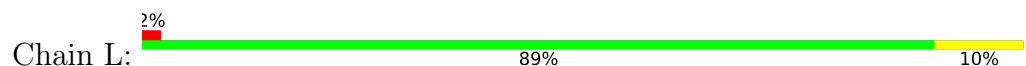
• Molecule 3: FAB 9C5 heavy chain



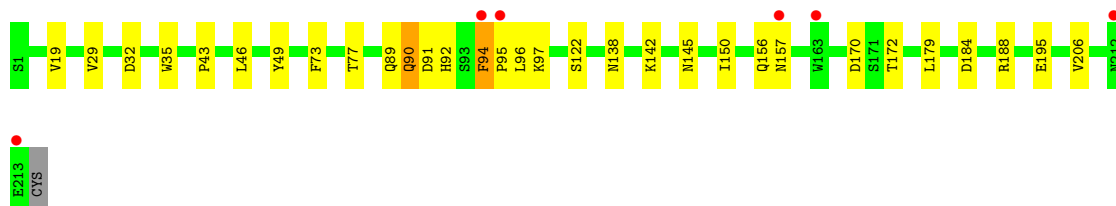
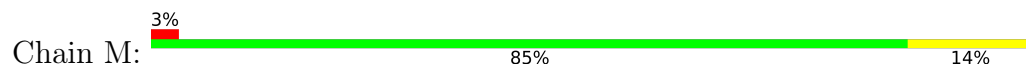
• Molecule 3: FAB 9C5 heavy chain



• Molecule 4: FAB 9C5 light chain



• Molecule 4: FAB 9C5 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.25Å 239.25Å 68.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.65 – 2.42 47.65 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.65-2.42) 92.0 (47.65-2.42)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.211 , 0.247 0.211 , 0.247	Depositor DCC
R_{free} test set	3827 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 70.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12718	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NA, EDO, CL, GOL

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	0.12	0/2568	0.28	0/3494
1	C	0.13	0/2583	0.28	0/3510
2	B	0.13	0/251	0.36	0/340
2	D	0.14	0/262	0.42	0/355
3	H	0.15	0/1660	0.35	0/2277
3	I	0.19	0/1658	0.37	0/2270
4	L	0.15	0/1687	0.36	0/2295
4	M	0.15	0/1681	0.36	0/2288
All	All	0.15	0/12350	0.33	0/16829

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2516	0	2391	31	0
1	C	2533	0	2421	21	0
2	B	244	0	244	7	0
2	D	255	0	244	7	0
3	H	1613	0	1553	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1612	0	1555	14	0
4	L	1646	0	1562	11	0
4	M	1643	0	1562	17	0
5	C	8	0	12	0	0
5	I	4	0	6	0	0
5	L	4	0	6	0	0
5	M	8	0	12	1	0
6	H	10	0	4	0	0
6	I	5	0	2	0	0
7	H	1	0	0	0	0
7	M	1	0	0	0	0
8	L	1	0	0	0	0
8	M	1	0	0	0	0
9	I	6	0	8	1	0
10	M	10	0	12	0	0
11	A	66	0	0	0	0
11	B	8	0	0	0	0
11	C	81	0	0	0	0
11	D	6	0	0	0	0
11	H	102	0	0	0	0
11	I	121	0	0	0	0
11	L	103	0	0	0	0
11	M	110	0	0	0	0
All	All	12718	0	11594	106	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 4.

All (106) 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)
3:I:120:VAL:H	9:I:303:GOL:H32	1.53	0.73
3:I:40:ARG:HG2	3:I:88:ALA:HB2	1.77	0.67
1:C:24:ASN:HB3	1:C:27:THR:HG23	1.77	0.66
3:I:188:PRO:HB3	3:I:211:PRO:HG3	1.80	0.63
1:A:24:ASN:HB3	1:A:27:THR:HG23	1.81	0.62
1:A:39:ARG:HE	1:A:265:ASN:HA	1.63	0.62
1:C:255:PRO:HG3	1:C:260:LEU:HD13	1.81	0.61
1:A:235:LEU:HD22	1:A:263:LEU:HD12	1.84	0.59
1:A:293:ILE:HD11	2:B:388:VAL:HG13	1.82	0.59
3:H:122:PRO:HD3	3:H:207:LYS:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LEU:HD22	1:C:181:VAL:HG22	1.86	0.57
1:C:218:VAL:HG12	2:D:392:THR:HG23	1.85	0.56
4:L:150:ILE:HD11	4:L:179:LEU:HD21	1.87	0.56
4:M:91:ASP:HA	4:M:96:LEU:HD22	1.87	0.56
1:A:291:LEU:HD12	1:A:340:ILE:HD12	1.89	0.55
1:A:118:LEU:HD11	1:A:182:PHE:HE1	1.71	0.54
1:A:121:SER:HB2	1:A:181:VAL:HG23	1.89	0.54
4:M:195:GLU:HG2	4:M:206:VAL:HG22	1.88	0.54
3:I:38:LYS:HB2	3:I:48:ILE:HD11	1.88	0.54
4:M:29:VAL:HG11	4:M:90:GLN:HG3	1.91	0.53
1:A:299:LEU:HD12	1:A:351:MET:HE1	1.90	0.53
1:C:318:LEU:HD22	1:C:327:LEU:HB3	1.90	0.53
2:D:369:PRO:HA	2:D:388:VAL:O	2.09	0.52
4:M:46:LEU:HD21	4:M:49:TYR:HB3	1.91	0.52
3:I:98:SER:HB2	5:M:501:EDO:H21	1.91	0.52
4:L:90:GLN:HG2	4:L:92:HIS:H	1.76	0.51
4:M:170:ASP:OD1	4:M:172[B]:THR:HG22	2.11	0.51
4:M:150:ILE:HD11	4:M:179:LEU:HD21	1.91	0.51
3:I:134:MET:HE3	3:I:181:THR:HG22	1.92	0.51
1:C:48:THR:HA	2:D:393:GLN:HE22	1.75	0.51
1:C:24:ASN:OD1	1:C:26:ILE:HG12	2.11	0.50
4:M:90:GLN:HG2	4:M:92:HIS:H	1.75	0.50
1:C:254:LEU:HD11	2:D:368:LYS:HG3	1.94	0.50
3:H:11:LEU:HD22	3:H:146:PRO:HG3	1.95	0.49
3:H:134:MET:HE3	3:H:181:THR:HG22	1.93	0.49
2:D:373:LEU:HD12	2:D:384:PHE:O	2.12	0.48
1:C:287:HIS:HB2	2:D:365:LYS:HA	1.95	0.48
1:A:63:MET:HE2	1:A:118:LEU:HD13	1.96	0.48
1:A:338:LEU:HD22	2:B:372:PHE:CZ	2.49	0.47
2:B:369:PRO:HA	2:B:388:VAL:O	2.15	0.47
1:A:268:THR:O	1:A:272:ILE:HG12	2.14	0.47
3:H:82(C):LEU:HA	3:H:86:ASP:OD2	2.14	0.47
4:M:142:LYS:HE2	4:M:142:LYS:HB3	1.52	0.47
1:C:226:MET:HB3	1:C:281:ARG:HB3	1.96	0.47
4:M:95:PRO:O	4:M:97:LYS:HG2	2.14	0.46
1:A:147:PHE:O	1:A:150:THR:HG22	2.15	0.46
1:C:28:PRO:HB3	1:C:269[A]:HIS:CD2	2.51	0.46
1:C:136:LYS:HD2	3:I:31:ASP:C	2.40	0.46
1:A:119:PHE:HB2	1:A:183:ALA:HB3	1.96	0.46
4:L:4:MET:HE3	4:L:23:CYS:SG	2.55	0.46
4:L:29:VAL:HG11	4:L:90:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLU:OE2	3:H:50:ARG:NH1	2.49	0.46
1:A:124:LEU:HD22	1:A:181:VAL:HG22	1.98	0.45
1:C:176:LEU:HD12	1:C:176:LEU:HA	1.81	0.45
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.98	0.45
3:H:12:VAL:HG21	3:H:82(C):LEU:HD12	1.98	0.45
4:M:184:ASP:O	4:M:188:ARG:HG3	2.16	0.45
1:C:288:LEU:HD12	1:C:289:PRO:HD2	1.98	0.45
1:C:239:VAL:HG21	1:C:275:PHE:CE2	2.52	0.45
1:C:39:ARG:HE	1:C:265:ASN:HA	1.82	0.44
3:I:20:LEU:HD22	3:I:106:THR:HG21	2.00	0.44
4:L:193:THR:HG23	4:L:206:VAL:HG13	1.99	0.44
1:A:55:VAL:HG23	2:B:382:PRO:O	2.17	0.44
3:H:150[B]:THR:OG1	3:H:197:ALA:HB3	2.17	0.44
1:A:114:THR:HG22	1:A:188:ILE:HG13	1.98	0.44
3:H:118:PRO:HB3	3:H:144:TYR:HB3	2.00	0.44
1:A:168:LYS:HE2	1:A:346:GLU:OE1	2.18	0.44
4:L:46:LEU:HD23	4:L:55:LYS:HD2	2.00	0.44
4:M:138:ASN:HA	4:M:172[B]:THR:CG2	2.48	0.44
3:H:35:HIS:NE2	3:H:50:ARG:HG3	2.33	0.43
1:A:267:LEU:HD22	1:A:272:ILE:HD11	2.00	0.43
1:A:118:LEU:HG	1:A:120:LEU:HD21	1.99	0.43
3:H:100:ASP:HA	4:L:46:LEU:HD22	2.00	0.43
3:I:183:PRO:HB2	3:I:186:THR:HG23	2.00	0.43
1:A:34:ALA:HB2	1:A:54:PRO:HB3	2.01	0.43
3:H:50:ARG:HE	3:H:50:ARG:C	2.27	0.43
4:L:32:ASP:HB3	4:L:91:ASP:OD1	2.18	0.43
1:C:268:THR:O	1:C:272:ILE:HG12	2.19	0.43
3:I:38:LYS:HE2	3:I:40:ARG:HH11	1.84	0.43
1:A:262:HIS:CD2	1:A:266:GLU:HG3	2.54	0.42
1:C:27:THR:HG21	2:D:379:THR:O	2.20	0.42
1:A:120:LEU:HD22	1:A:126:LEU:HD21	2.01	0.42
1:A:157:ILE:HG23	1:A:185:VAL:HG21	2.00	0.42
1:C:51:PHE:CZ	1:C:338:LEU:HB2	2.55	0.42
4:L:195:GLU:HG3	4:L:204:PRO:HB2	2.02	0.42
1:A:27:THR:HG21	2:B:379:THR:O	2.19	0.42
1:C:231:HIS:HD2	1:C:238:TRP:CD1	2.38	0.41
3:I:58:LYS:HZ3	4:M:94:PHE:HE2	1.67	0.41
1:A:343:LYS:HE3	1:A:343:LYS:HB2	1.76	0.41
3:I:103:GLY:O	4:M:43:PRO:HB3	2.20	0.41
1:A:121:SER:HA	1:A:145:VAL:O	2.20	0.41
3:H:126:GLY:HA2	3:H:212:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:89:GLN:HG3	4:L:98:PHE:CE2	2.56	0.41
1:A:209:HIS:O	2:B:369:PRO:HD3	2.21	0.41
2:B:375:ILE:HD13	2:B:382:PRO:HA	2.03	0.41
1:A:27:THR:OG1	1:A:28:PRO:HD3	2.21	0.40
1:C:299:LEU:HD12	1:C:351:MET:HE1	2.01	0.40
3:H:20:LEU:HD22	3:H:106:THR:HG21	2.03	0.40
4:L:13:VAL:HG22	4:L:14:SER:O	2.21	0.40
3:I:58:LYS:NZ	4:M:94:PHE:HE2	2.19	0.40
3:I:104:GLN:HA	4:M:43:PRO:HB3	2.03	0.40
4:M:35:TRP:CE2	4:M:73:PHE:HB2	2.56	0.40
1:A:38:TYR:HE2	1:A:264:GLU:HG2	1.85	0.40
3:H:82:LEU:HB3	3:H:82(C):LEU:HD21	2.04	0.40
1:A:24:ASN:OD1	1:A:26:ILE:HG12	2.22	0.40
4:M:32:ASP:HB3	4:M:91:ASP:OD1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/364 (91%)	330 (99%)	2 (1%)	0	100	100
1	C	331/364 (91%)	327 (99%)	4 (1%)	0	100	100
2	B	30/40 (75%)	29 (97%)	1 (3%)	0	100	100
2	D	31/40 (78%)	30 (97%)	1 (3%)	0	100	100
3	H	218/218 (100%)	215 (99%)	3 (1%)	0	100	100
3	I	213/218 (98%)	211 (99%)	2 (1%)	0	100	100
4	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
4	M	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
All	All	1579/1672 (94%)	1553 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	257/319 (81%)	252 (98%)	5 (2%)	50	70
1	C	264/319 (83%)	262 (99%)	2 (1%)	73	85
2	B	27/38 (71%)	27 (100%)	0	100	100
2	D	28/38 (74%)	28 (100%)	0	100	100
3	H	179/188 (95%)	170 (95%)	9 (5%)	22	36
3	I	181/188 (96%)	175 (97%)	6 (3%)	33	53
4	L	185/190 (97%)	180 (97%)	5 (3%)	39	60
4	M	183/190 (96%)	174 (95%)	9 (5%)	22	37
All	All	1304/1470 (89%)	1268 (97%)	36 (3%)	38	58

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	210	VAL
1	A	213	VAL
1	A	301	SER
1	A	303	LEU
1	C	145	VAL
1	C	159	ASP
3	H	40	ARG
3	H	43	GLN
3	H	50	ARG
3	H	58	LYS
3	H	94	ARG
3	H	112	SER
3	H	169	LEU
3	H	176	LEU
3	H	207	LYS

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Mol	Chain	Res	Type
4	L	77	THR
4	L	90	GLN
4	L	94	PHE
4	L	96	LEU
4	L	213	GLU
3	I	5	GLN
3	I	50	ARG
3	I	94	ARG
3	I	139	CYS
3	I	176	LEU
3	I	194	CYS
4	M	19	VAL
4	M	77	THR
4	M	89	GLN
4	M	90	GLN
4	M	94	PHE
4	M	122	SER
4	M	145	ASN
4	M	156	GLN
4	M	157	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	81	ASN
1	A	262	HIS
1	C	109	GLN
1	C	278	ASN
1	C	287	HIS
3	H	39	GLN
4	L	38	GLN
4	L	53	ASN
4	L	79	GLN
3	I	5	GLN
3	I	39	GLN
4	M	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EDO	I	302	-	3,3,3	0.26	0	2,2,2	0.26	0
5	EDO	M	502	-	3,3,3	0.28	0	2,2,2	0.08	0
5	EDO	M	501	-	3,3,3	0.25	0	2,2,2	0.41	0
6	GLY	H	302	-	4,4,4	1.16	1 (25%)	3,4,4	1.77	2 (66%)
9	GOL	I	303	-	5,5,5	0.35	0	5,5,5	0.54	0
5	EDO	L	401	-	3,3,3	0.25	0	2,2,2	0.18	0
10	LYS	M	503	-	8,9,9	0.79	1 (12%)	7,10,10	0.95	1 (14%)
5	EDO	C	401	-	3,3,3	0.24	0	2,2,2	0.43	0
6	GLY	I	301	-	4,4,4	1.05	1 (25%)	3,4,4	1.89	2 (66%)
6	GLY	H	301	-	4,4,4	1.15	1 (25%)	3,4,4	1.64	1 (33%)
5	EDO	C	402	-	3,3,3	0.25	0	2,2,2	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	I	302	-	-	1/1/1/1	-
5	EDO	M	502	-	-	0/1/1/1	-
5	EDO	M	501	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GLY	H	302	-	-	2/2/2/2	-
9	GOL	I	303	-	-	2/4/4/4	-
5	EDO	L	401	-	-	0/1/1/1	-
10	LYS	M	503	-	-	1/9/9/9	-
5	EDO	C	401	-	-	1/1/1/1	-
6	GLY	I	301	-	-	2/2/2/2	-
6	GLY	H	301	-	-	2/2/2/2	-
5	EDO	C	402	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	302	GLY	OXT-C	-2.22	1.23	1.30
6	H	301	GLY	OXT-C	-2.17	1.23	1.30
10	M	503	LYS	OXT-C	-2.09	1.24	1.30
6	I	301	GLY	OXT-C	-2.02	1.24	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	503	LYS	OXT-C-O	-2.43	118.57	124.08
6	I	301	GLY	OXT-C-CA	2.34	122.68	113.38
6	H	302	GLY	OXT-C-O	-2.29	117.45	123.33
6	I	301	GLY	OXT-C-O	-2.21	117.65	123.33
6	H	301	GLY	OXT-C-CA	2.03	121.46	113.38
6	H	302	GLY	OXT-C-CA	2.01	121.39	113.38

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	302	GLY	O-C-CA-N
6	I	301	GLY	O-C-CA-N
6	I	301	GLY	OXT-C-CA-N
9	I	303	GOL	O1-C1-C2-C3
6	H	302	GLY	OXT-C-CA-N
5	C	401	EDO	O1-C1-C2-O2
9	I	303	GOL	O1-C1-C2-O2
5	M	501	EDO	O1-C1-C2-O2
6	H	301	GLY	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
6	H	301	GLY	O-C-CA-N
5	I	302	EDO	O1-C1-C2-O2
10	M	503	LYS	OXT-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	501	EDO	1	0
9	I	303	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	332/364 (91%)	0.67	19 (5%)	29 25	35, 63, 95, 122	2 (0%)
1	C	332/364 (91%)	0.53	21 (6%)	26 22	33, 56, 98, 119	1 (0%)
2	B	32/40 (80%)	0.42	2 (6%)	26 22	43, 52, 75, 78	0
2	D	33/40 (82%)	0.65	2 (6%)	27 23	46, 60, 93, 104	0
3	H	217/218 (99%)	-0.09	9 (4%)	41 37	17, 34, 71, 124	3 (1%)
3	I	214/218 (98%)	-0.02	5 (2%)	61 57	15, 36, 62, 117	3 (1%)
4	L	213/214 (99%)	0.11	5 (2%)	61 57	21, 42, 68, 93	1 (0%)
4	M	213/214 (99%)	-0.02	6 (2%)	55 51	14, 39, 60, 94	1 (0%)
All	All	1586/1672 (94%)	0.27	69 (4%)	39 34	14, 47, 90, 124	11 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	94	PHE	4.9
3	H	213	ASP	4.7
3	H	131	THR	4.4
4	M	94	PHE	4.4
2	D	362	PRO	4.0
1	C	199	GLU	3.9
3	I	128	GLY	3.9
1	C	213	VAL	3.7
1	A	47	SER	3.7
1	A	293	ILE	3.6
3	I	213	ASP	3.4
3	I	127	SER	3.3
3	H	127	SER	3.2
1	A	178	ARG	3.2
4	M	212	ASN	3.1
1	A	176	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	280	ASP	3.0
1	C	269[A]	HIS	2.9
1	A	177	ASP	2.9
3	H	126	GLY	2.9
3	H	129	ALA	2.8
1	C	280	ASP	2.8
3	I	126	GLY	2.7
1	A	182	PHE	2.7
1	A	354	GLU	2.7
3	H	130	GLN	2.6
1	C	178	ARG	2.6
1	C	238	TRP	2.5
1	C	200	VAL	2.5
1	A	148	GLY	2.5
3	H	128	GLY	2.5
4	L	212	ASN	2.5
3	I	42	GLU	2.5
1	C	204	GLU	2.4
1	C	229	ILE	2.4
1	A	23	PHE	2.4
4	L	202	THR	2.4
1	A	152	GLU	2.4
1	C	282	ARG	2.4
2	B	362	PRO	2.4
1	C	236	SER	2.4
1	A	261[A]	GLN	2.4
2	D	364	VAL	2.4
1	C	230	GLN	2.3
1	A	325	ALA	2.3
4	M	163	TRP	2.3
1	A	282	ARG	2.3
3	H	41	PRO	2.3
1	C	108	SER	2.3
1	A	327	LEU	2.3
1	C	224	LEU	2.3
1	A	329	LEU	2.3
1	A	175	GLU	2.3
2	B	364	VAL	2.3
1	A	153	ALA	2.2
4	L	203	SER	2.2
4	M	157	ASN	2.2
1	C	275	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	259	LYS	2.2
1	C	326	PRO	2.2
1	A	158	ASN	2.1
3	H	42	GLU	2.1
1	C	245	LEU	2.1
4	M	95	PRO	2.1
4	M	213	GLU	2.1
1	C	234	LYS	2.1
4	L	95	PRO	2.0
1	C	227	PHE	2.0
1	C	176	LEU	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 oligosaccharides 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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	M	502	4/4	0.71	0.24	46,48,51,56	0
6	GLY	I	301	5/5	0.71	0.23	55,55,56,56	0
10	LYS	M	503	10/10	0.82	0.17	65,66,68,68	0
6	GLY	H	302	5/5	0.87	0.15	56,57,57,60	0
5	EDO	L	401	4/4	0.88	0.14	44,44,44,44	0
5	EDO	C	401	4/4	0.89	0.13	45,49,50,54	0
7	CL	H	303	1/1	0.90	0.09	66,66,66,66	0
9	GOL	I	303	6/6	0.90	0.15	29,36,40,46	0
5	EDO	C	402	4/4	0.90	0.11	47,48,50,51	0
5	EDO	I	302	4/4	0.91	0.12	38,39,44,45	0
6	GLY	H	301	5/5	0.92	0.09	44,45,45,45	0
5	EDO	M	501	4/4	0.92	0.12	42,43,43,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NA	L	402	1/1	0.93	0.15	45,45,45,45	0
8	NA	M	505	1/1	0.93	0.25	53,53,53,53	0
7	CL	M	504	1/1	0.96	0.07	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.