



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:49 PM UTC

PDB ID : 8EN5 / pdb_00008en5
Title : Structure of GII.4 norovirus in complex with Nanobody 56
Authors : Kher, G.; Sabin, C.; Pancera, M.; Koromyslova, A.; Hansman, G.
Deposited on : 2022-09-28
Resolution : 1.60 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

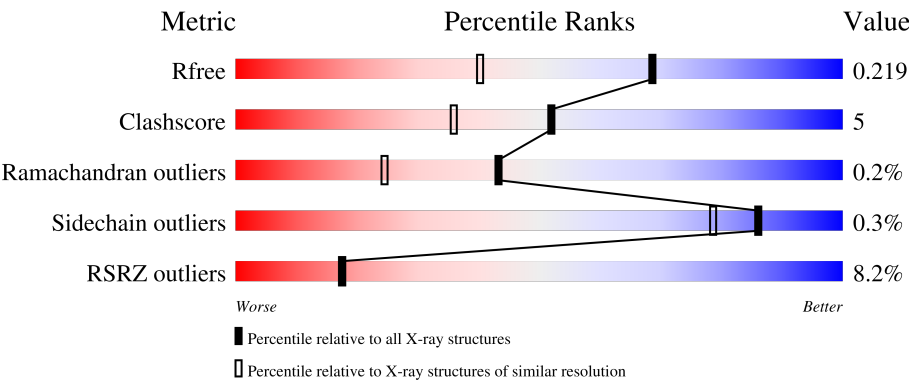
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	317	
1	B	317	
1	C	317	
1	D	317	
2	E	131	

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Mol	Chain	Length	Quality of chain
2	F	131	
2	G	131	
2	H	131	

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
3	EDO	B	606	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15074 atoms, of which 36 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 GII.4 P domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	2	0
			2418	1532	415	461	10			
1	B	308	Total	C	N	O	S	0	3	0
			2427	1540	415	462	10			
1	C	308	Total	C	N	O	S	0	0	0
			2406	1524	412	460	10			
1	D	306	Total	C	N	O	S	0	0	0
			2395	1518	410	457	10			

- Molecule 2 is a protein called Nanobody 56.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	126	Total	C	N	O	S	0	0	0
			973	611	170	188	4			
2	F	125	Total	C	N	O	S	0	0	0
			963	605	167	187	4			
2	G	131	Total	C	N	O	S	0	1	0
			1026	643	185	194	4			
2	H	124	Total	C	N	O	S	0	0	0
			957	602	166	185	4			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	O		0	0
			4	2	2			
3	B	1	Total	C	O		0	0
			4	2	2			
3	B	1	Total	C	O		0	0
			4	2	2			
3	B	1	Total	C	O		0	0
			4	2	2			
3	B	1	Total	C	O		0	0
			4	2	2			

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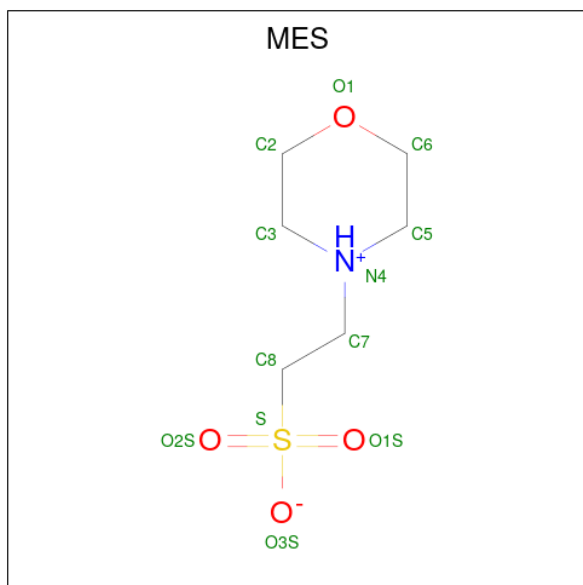
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O		0	0
			4	2	2			
3	B	1	Total	C	O		0	0
			4	2	2			
3	B	1	Total	C	O		0	0
			4	2	2			
3	B	1	Total	C	O		0	0
			4	2	2			
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	E	1	Total	C	H	O	0	0
			10	2	6	2		
3	F	1	Total	C	O		0	0
			4	2	2			
3	F	1	Total	C	O		0	0
			4	2	2			
3	F	1	Total	C	O		0	0
			4	2	2			
3	C	1	Total	C	O		0	0
			4	2	2			
3	C	1	Total	C	O		0	0
			4	2	2			
3	C	1	Total	C	O		0	0
			4	2	2			
3	C	1	Total	C	O		0	0
			4	2	2			
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	O		0	0
			4	2	2			
3	D	1	Total	C	O		0	0
			4	2	2			
3	D	1	Total	C	O		0	0
			4	2	2			
3	D	1	Total	C	O		0	0
			4	2	2			
3	G	1	Total	C	O		0	0
			4	2	2			

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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	322	Total	O	0	0
			322	322		
5	B	278	Total	O	0	0
			278	278		
5	E	83	Total	O	0	0
			83	83		
5	F	95	Total	O	0	0
			95	95		
5	C	238	Total	O	0	0
			238	238		
5	D	166	Total	O	0	0
			166	166		
5	G	69	Total	O	0	0
			69	69		

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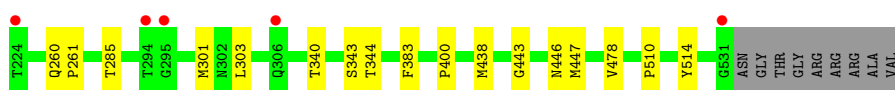
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	66	Total	O	0	0
			66	66		

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.

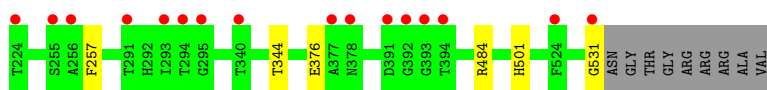
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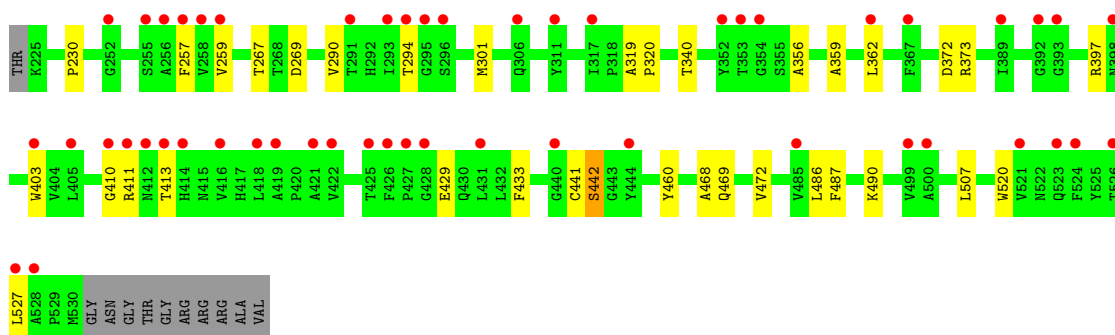
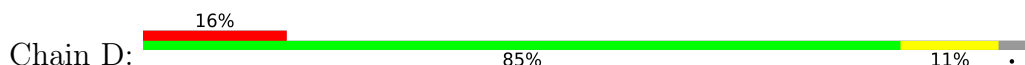
- Molecule 1: GII.4 P domain



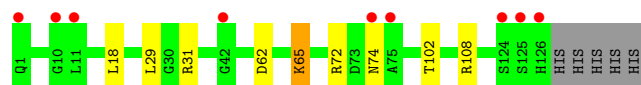
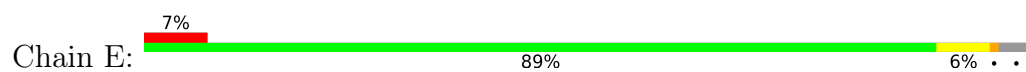
- Molecule 1: GII.4 P domain



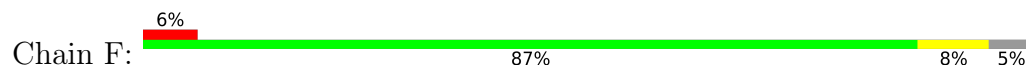
- Molecule 1: GII.4 P domain



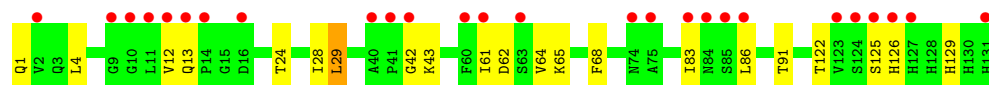
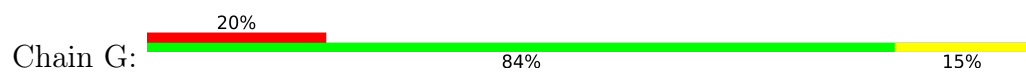
- Molecule 2: Nanobody 56



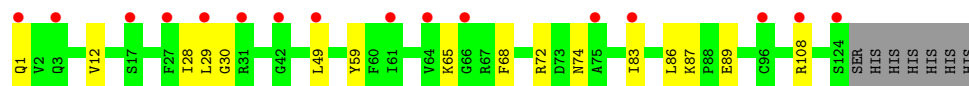
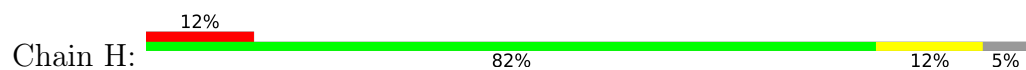
• Molecule 2: Nanobody 56



• Molecule 2: Nanobody 56



• Molecule 2: Nanobody 56



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.24Å 235.38Å 70.57Å 90.00° 104.30° 90.00°	Depositor
Resolution (Å)	68.38 – 1.60 68.38 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.4 (68.38-1.60) 92.8 (68.38-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.219 0.186 , 0.219	Depositor DCC
R_{free} test set	12382 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15074	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 3.44% 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

5.1 Standard geometry

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

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	0.73	0/2494	0.76	0/3411
1	B	0.74	0/2507	0.77	0/3429
1	C	0.60	0/2476	0.67	0/3387
1	D	0.50	0/2465	0.61	0/3372
2	E	0.58	0/994	0.73	0/1348
2	F	0.61	0/983	0.72	0/1333
2	G	0.47	0/1055	0.63	0/1431
2	H	0.48	0/977	0.65	0/1325
All	All	0.62	0/13951	0.70	0/19036

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	410	ARG	Peptide

5.2 Too-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 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	2418	0	2322	14	0
1	B	2427	0	2331	13	0
1	C	2406	0	2302	9	0
1	D	2395	0	2292	30	0
2	E	973	0	944	9	0
2	F	963	0	937	21	0
2	G	1026	0	984	24	0
2	H	957	0	932	24	0
3	A	32	6	48	6	0
3	B	52	18	78	8	0
3	C	20	6	30	3	0
3	D	16	0	24	3	0
3	E	4	6	6	0	0
3	F	12	0	18	2	0
3	G	4	0	6	1	0
3	H	4	0	6	1	0
4	A	12	0	12	0	0
5	A	322	0	0	3	0
5	B	278	0	0	3	0
5	C	238	0	0	4	0
5	D	166	0	0	1	0
5	E	83	0	0	0	0
5	F	95	0	0	2	0
5	G	69	0	0	0	0
5	H	66	0	0	2	0
All	All	15038	36	13272	138	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 5.

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:ARG:HH11	2:F:72:ARG:HD2	1.11	1.15
2:H:72:ARG:HD3	2:H:74:ASN:HD21	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:125:SER:O	2:G:129:HIS:NE2	2.03	0.90
1:C:501:HIS:CE1	1:C:531:GLY:HA3	2.09	0.86
2:F:31:ARG:NH1	2:F:72:ARG:HD2	1.92	0.85
2:F:31:ARG:HD3	2:F:74:ASN:OD1	1.75	0.85
1:D:257:PHE:HZ	3:D:602:EDO:H22	1.42	0.84
1:D:372:ASP:OD1	1:D:373:ARG:NH1	2.12	0.82
1:C:376:GLU:HG2	5:C:891:HOH:O	1.80	0.80
2:E:108:ARG:HH11	2:E:108:ARG:HG2	1.45	0.80
2:F:31:ARG:CD	2:F:74:ASN:HD21	1.96	0.78
2:G:13:GLN:NE2	2:G:126:HIS:H	1.82	0.77
2:E:62:ASP:OD1	2:E:65:LYS:HE3	1.86	0.75
2:F:31:ARG:HD3	2:F:74:ASN:CG	2.11	0.75
2:H:72:ARG:CD	2:H:74:ASN:HD21	1.99	0.75
2:F:31:ARG:HD3	2:F:74:ASN:ND2	2.02	0.75
3:C:604:EDO:H11	5:C:905:HOH:O	1.87	0.74
1:A:443:GLY:H	3:B:606:EDO:H12	1.53	0.74
1:D:340:THR:HG23	5:D:828:HOH:O	1.91	0.70
1:B:285[A]:THR:HG23	5:B:706:HOH:O	1.91	0.70
2:F:31:ARG:HD3	2:F:74:ASN:HD21	1.54	0.69
1:D:472:VAL:HG11	1:D:490:LYS:HD3	1.73	0.69
1:D:469:GLN:HB2	1:D:520:TRP:CD1	2.27	0.68
3:A:609:EDO:H11	5:A:925:HOH:O	1.93	0.67
1:B:329:LYS:HG2	1:B:352[B]:TYR:CD1	2.29	0.67
1:D:486:LEU:HD23	1:D:487:PHE:HD1	1.61	0.65
2:G:13:GLN:NE2	2:G:126:HIS:HB2	2.13	0.64
1:A:443:GLY:H	3:B:606:EDO:C1	2.12	0.63
2:G:13:GLN:HE21	2:G:126:HIS:CG	2.17	0.62
2:G:91:THR:HG23	2:G:122:THR:HA	1.80	0.62
1:A:343:SER:HB2	3:A:604:EDO:H22	1.81	0.62
1:D:486:LEU:HG	2:H:29:LEU:HD22	1.81	0.62
1:C:501:HIS:ND1	1:C:531:GLY:HA3	2.15	0.61
1:D:429:GLU:OE2	1:D:490:LYS:NZ	2.31	0.61
1:A:510:PRO:HD3	3:A:603:EDO:H12	1.84	0.60
1:D:257:PHE:CZ	3:D:602:EDO:H22	2.30	0.60
2:E:72:ARG:HD2	2:E:74:ASN:OD1	2.02	0.59
1:C:484:ARG:HD2	3:C:604:EDO:O2	2.03	0.59
2:G:125:SER:C	2:G:129:HIS:HE2	2.10	0.59
2:F:31:ARG:HH11	2:F:72:ARG:CD	1.99	0.59
2:H:68:PHE:CE1	2:H:83:ILE:HG23	2.38	0.59
2:G:61:ILE:O	2:G:64:VAL:HG22	2.03	0.59
3:A:609:EDO:C1	5:A:925:HOH:O	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:18:LEU:HD12	2:E:18:LEU:C	2.28	0.57
2:H:68:PHE:CE2	2:H:83:ILE:HD13	2.40	0.57
1:A:344:THR:O	3:A:604:EDO:H21	2.05	0.57
1:D:486:LEU:HD23	1:D:487:PHE:CD1	2.40	0.57
2:F:31:ARG:CZ	2:F:74:ASN:HD21	2.19	0.56
2:E:108:ARG:HG2	2:E:108:ARG:NH1	2.16	0.56
2:H:30:GLY:HA2	3:H:201:EDO:H21	1.89	0.55
2:G:13:GLN:HE22	2:G:126:HIS:HB2	1.71	0.55
1:D:441:CYS:O	1:D:442:SER:HB3	2.06	0.55
2:F:31:ARG:NE	2:F:74:ASN:HD21	2.05	0.54
1:D:359:ALA:HB1	1:D:362:LEU:HD12	1.90	0.54
1:A:340:THR:HG23	5:A:904:HOH:O	2.08	0.53
2:G:13:GLN:NE2	2:G:126:HIS:CB	2.72	0.53
1:D:319:ALA:HB1	1:D:320:PRO:HD2	1.91	0.52
2:E:72:ARG:CD	2:E:74:ASN:OD1	2.57	0.52
1:B:505:ASP:H	2:F:1:GLN:N	2.08	0.52
2:G:68:PHE:CE1	2:G:83:ILE:HG12	2.45	0.51
1:A:438:MET:O	1:A:447:MET:HG2	2.10	0.50
2:H:68:PHE:CZ	2:H:83:ILE:HD13	2.46	0.50
2:H:83:ILE:CG2	2:H:86:LEU:HD21	2.42	0.50
1:D:469:GLN:HB2	1:D:520:TRP:CG	2.46	0.50
1:D:397:ARG:HG3	1:D:397:ARG:NH1	2.27	0.49
2:G:4:LEU:HD22	2:G:24:THR:HG22	1.94	0.49
2:H:49:LEU:HD21	2:H:59:TYR:CE2	2.47	0.49
2:F:31:ARG:CD	2:F:74:ASN:ND2	2.67	0.49
2:G:83:ILE:HG21	2:G:86:LEU:HD23	1.93	0.49
1:A:478:VAL:CG2	1:A:514:TYR:CE1	2.96	0.48
1:D:230:PRO:HD3	1:D:460:TYR:CD2	2.48	0.48
1:C:531:GLY:O	5:C:701:HOH:O	2.20	0.48
2:F:34:ILE:HD13	2:F:98:ALA:HB2	1.95	0.47
2:F:27:PHE:HE1	3:F:202:EDO:H11	1.79	0.47
1:B:486:PHE:CD2	1:B:529:MET:HE1	2.49	0.47
5:C:803:HOH:O	2:H:108:ARG:HD3	2.14	0.47
1:D:290:VAL:HG12	1:D:301:MET:HB2	1.97	0.47
1:D:410:GLY:O	1:D:413:THR:OG1	2.30	0.47
1:A:478:VAL:HG23	1:A:514:TYR:CE1	2.50	0.47
2:H:87:LYS:HE3	2:H:89:GLU:OE1	2.15	0.47
2:G:125:SER:O	2:G:129:HIS:CD2	2.68	0.46
2:H:29:LEU:HD23	2:H:29:LEU:HA	1.74	0.46
2:H:72:ARG:HD3	2:H:74:ASN:ND2	2.16	0.46
1:B:258:VAL:CG1	3:B:610:EDO:H11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:603:EDO:H11	2:E:102:THR:HG21	1.98	0.46
1:B:402:TRP:O	3:B:610:EDO:H22	2.16	0.46
2:F:41:PRO:HD3	5:F:363:HOH:O	2.16	0.46
1:D:469:GLN:NE2	1:D:469:GLN:HA	2.31	0.45
2:G:29:LEU:O	3:G:201:EDO:H21	2.16	0.45
2:F:72:ARG:HG3	3:F:201:EDO:H11	1.98	0.45
1:C:344:THR:O	1:D:442:SER:HA	2.17	0.45
3:B:613:EDO:C2	5:B:707:HOH:O	2.65	0.44
1:D:490:LYS:HG3	1:D:527:LEU:HD11	2.00	0.44
1:B:425:PHE:HE2	1:B:523:PHE:HA	1.82	0.44
2:H:49:LEU:HD21	2:H:59:TYR:CZ	2.52	0.44
2:E:65:LYS:HE2	2:E:65:LYS:HB3	1.24	0.44
3:B:609:EDO:H22	5:B:837:HOH:O	2.17	0.43
2:G:62:ASP:O	2:G:65:LYS:HB2	2.18	0.43
1:A:301:MET:HG2	1:A:303:LEU:HD23	1.99	0.43
1:A:443:GLY:N	3:B:606:EDO:H12	2.28	0.43
1:C:531:GLY:HA2	2:G:28:ILE:CG2	2.48	0.43
1:D:507:LEU:HD23	2:H:29:LEU:CD1	2.49	0.43
2:F:74:ASN:HB2	5:F:351:HOH:O	2.18	0.43
2:H:1:GLN:N	5:H:307:HOH:O	2.52	0.43
2:H:83:ILE:HG22	2:H:86:LEU:HD21	2.00	0.43
1:A:400:PRO:HD2	1:A:446:ASN:O	2.19	0.43
2:H:12:VAL:HG21	2:H:86:LEU:HD13	2.00	0.43
1:B:530:GLY:HA2	2:F:28:ILE:HB	2.00	0.42
1:C:531:GLY:HA2	2:G:28:ILE:HG21	2.01	0.42
1:A:260:GLN:N	1:A:261:PRO:CD	2.81	0.42
2:G:13:GLN:HE22	2:G:126:HIS:H	1.62	0.42
1:D:259:VAL:HG13	1:D:403:TRP:CZ3	2.54	0.42
1:D:486:LEU:CG	2:H:29:LEU:HD22	2.48	0.42
2:G:64:VAL:HB	2:G:68:PHE:CG	2.55	0.42
1:D:433:PHE:CE2	3:D:602:EDO:H21	2.55	0.42
1:D:468:ALA:HA	1:D:520:TRP:CZ2	2.54	0.41
2:G:13:GLN:NE2	2:G:126:HIS:N	2.60	0.41
1:B:344:THR:O	3:B:606:EDO:H12	2.19	0.41
2:H:65:LYS:NZ	5:H:301:HOH:O	2.40	0.41
1:B:500:HIS:HB2	1:B:529:MET:HG2	2.01	0.41
1:D:507:LEU:HD23	2:H:29:LEU:HD12	2.01	0.41
2:F:31:ARG:HD2	2:F:72:ARG:CD	2.51	0.41
1:A:285[B]:THR:HG23	1:A:383:PHE:O	2.20	0.41
1:C:257:PHE:HZ	3:C:601:EDO:H11	1.86	0.41
1:D:319:ALA:HB1	1:D:320:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:42:GLY:O	2:G:43:LYS:HG2	2.20	0.41
2:G:12:VAL:CG2	2:G:86:LEU:HD13	2.51	0.41
2:G:43:LYS:HA	2:G:43:LYS:HD3	1.82	0.41
2:H:86:LEU:HD23	2:H:86:LEU:HA	1.95	0.41
1:B:327:VAL:HA	1:B:353:THR:OG1	2.21	0.40
1:B:508:ILE:O	2:F:101:PHE:HA	2.21	0.40
2:H:72:ARG:CD	2:H:74:ASN:ND2	2.76	0.40
1:D:267:THR:OG1	1:D:269:ASP:OD1	2.38	0.40
1:D:356:ALA:HA	1:D:411:ARG:HB2	2.02	0.40
1:B:505:ASP:N	2:F:1:GLN:N	2.69	0.40
2:E:31:ARG:HD3	2:E:74:ASN:OD1	2.22	0.40
2:G:13:GLN:NE2	2:G:126:HIS:CG	2.88	0.40
2:H:28:ILE:O	2:H:29:LEU:HB2	2.21	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	308/317 (97%)	303 (98%)	5 (2%)	0	100	100
1	B	309/317 (98%)	301 (97%)	8 (3%)	0	100	100
1	C	306/317 (96%)	300 (98%)	6 (2%)	0	100	100
1	D	304/317 (96%)	299 (98%)	4 (1%)	1 (0%)	36	20
2	E	124/131 (95%)	116 (94%)	7 (6%)	1 (1%)	16	5
2	F	123/131 (94%)	119 (97%)	3 (2%)	1 (1%)	16	5
2	G	130/131 (99%)	124 (95%)	5 (4%)	1 (1%)	16	5
2	H	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
All	All	1726/1792 (96%)	1680 (97%)	42 (2%)	4 (0%)	43	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	29	LEU
2	F	29	LEU
2	G	29	LEU
1	D	442	SER

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	269/273 (98%)	269 (100%)	0	100	100
1	B	270/273 (99%)	269 (100%)	1 (0%)	84	75
1	C	267/273 (98%)	267 (100%)	0	100	100
1	D	266/273 (97%)	265 (100%)	1 (0%)	84	75
2	E	105/110 (96%)	104 (99%)	1 (1%)	68	50
2	F	104/110 (94%)	104 (100%)	0	100	100
2	G	111/110 (101%)	110 (99%)	1 (1%)	70	55
2	H	103/110 (94%)	103 (100%)	0	100	100
All	All	1495/1532 (98%)	1491 (100%)	4 (0%)	86	78

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	522	GLN
2	E	65	LYS
1	D	294	THR
2	G	1	GLN

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	302	ASN

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Mol	Chain	Res	Type
1	A	504	GLN
2	E	3	GLN
2	E	13	GLN
2	F	13	GLN
2	F	74	ASN
1	C	469	GLN
1	C	504	GLN
1	D	469	GLN
2	G	13	GLN
2	H	5	GLN
2	H	74	ASN
2	H	93	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

37 ligands are modelled in this entry.

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	A	607	-	3,3,3	0.52	0	2,2,2	0.38	0
3	EDO	B	602	-	3,3,3	0.47	0	2,2,2	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	603	-	3,3,3	0.64	0	2,2,2	0.08	0
3	EDO	G	201	-	3,3,3	0.43	0	2,2,2	0.40	0
3	EDO	B	606	-	3,3,3	0.57	0	2,2,2	0.92	0
3	EDO	D	602	-	3,3,3	0.54	0	2,2,2	0.23	0
3	EDO	B	612	-	3,3,3	0.40	0	2,2,2	0.77	0
3	EDO	H	201	-	3,3,3	0.42	0	2,2,2	0.40	0
3	EDO	A	603	-	3,3,3	0.33	0	2,2,2	0.84	0
3	EDO	A	601	-	3,3,3	0.48	0	2,2,2	0.48	0
3	EDO	A	602	-	3,3,3	0.62	0	2,2,2	0.36	0
3	EDO	D	604	-	3,3,3	0.53	0	2,2,2	0.36	0
3	EDO	B	611	-	3,3,3	0.90	0	2,2,2	0.48	0
3	EDO	F	203	-	3,3,3	0.55	0	2,2,2	0.11	0
3	EDO	A	609	-	3,3,3	0.45	0	2,2,2	1.19	0
3	EDO	D	601	-	3,3,3	0.58	0	2,2,2	0.19	0
3	EDO	B	603	-	3,3,3	0.51	0	2,2,2	0.58	0
3	EDO	B	613	-	3,3,3	0.41	0	2,2,2	1.49	0
3	EDO	F	202	-	3,3,3	0.44	0	2,2,2	0.72	0
3	EDO	D	603	-	3,3,3	0.53	0	2,2,2	0.36	0
3	EDO	F	201	-	3,3,3	0.41	0	2,2,2	0.72	0
3	EDO	B	609	-	3,3,3	0.57	0	2,2,2	0.29	0
3	EDO	C	601	-	3,3,3	0.55	0	2,2,2	0.30	0
3	EDO	A	605	-	3,3,3	0.72	0	2,2,2	0.29	0
3	EDO	B	605	-	3,3,3	0.60	0	2,2,2	0.92	0
3	EDO	B	608	-	3,3,3	0.40	0	2,2,2	0.60	0
3	EDO	A	606	-	3,3,3	0.42	0	2,2,2	0.54	0
4	MES	A	608	-	12,12,12	1.94	1 (8%)	15,16,16	2.14	5 (33%)
3	EDO	C	602	-	3,3,3	0.48	0	2,2,2	0.61	0
3	EDO	C	605	-	3,3,3	0.43	0	2,2,2	0.50	0
3	EDO	E	201	-	3,3,3	0.37	0	2,2,2	0.50	0
3	EDO	B	610	-	3,3,3	0.44	0	2,2,2	0.30	0
3	EDO	C	604	-	3,3,3	0.38	0	2,2,2	0.33	0
3	EDO	B	607	-	3,3,3	0.68	0	2,2,2	0.21	0
3	EDO	B	601	-	3,3,3	0.58	0	2,2,2	0.52	0
3	EDO	A	604	-	3,3,3	0.54	0	2,2,2	0.32	0
3	EDO	B	604	-	3,3,3	0.45	0	2,2,2	0.53	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	A	607	-	-	0/1/1/1	-
3	EDO	B	602	-	-	0/1/1/1	-
3	EDO	C	603	-	-	0/1/1/1	-
3	EDO	G	201	-	-	1/1/1/1	-
3	EDO	B	606	-	-	1/1/1/1	-
3	EDO	D	602	-	-	1/1/1/1	-
3	EDO	B	612	-	-	1/1/1/1	-
3	EDO	H	201	-	-	1/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-
3	EDO	A	601	-	-	0/1/1/1	-
3	EDO	A	602	-	-	0/1/1/1	-
3	EDO	D	604	-	-	1/1/1/1	-
3	EDO	B	611	-	-	0/1/1/1	-
3	EDO	F	203	-	-	0/1/1/1	-
3	EDO	A	609	-	-	1/1/1/1	-
3	EDO	D	601	-	-	0/1/1/1	-
3	EDO	B	603	-	-	0/1/1/1	-
3	EDO	B	613	-	-	1/1/1/1	-
3	EDO	F	202	-	-	1/1/1/1	-
3	EDO	D	603	-	-	0/1/1/1	-
3	EDO	F	201	-	-	0/1/1/1	-
3	EDO	B	609	-	-	0/1/1/1	-
3	EDO	C	601	-	-	0/1/1/1	-
3	EDO	A	605	-	-	1/1/1/1	-
3	EDO	B	605	-	-	0/1/1/1	-
3	EDO	B	608	-	-	1/1/1/1	-
3	EDO	A	606	-	-	0/1/1/1	-
4	MES	A	608	-	-	5/6/14/14	0/1/1/1
3	EDO	C	602	-	-	0/1/1/1	-
3	EDO	C	605	-	-	0/1/1/1	-
3	EDO	E	201	-	-	0/1/1/1	-
3	EDO	B	610	-	-	1/1/1/1	-
3	EDO	C	604	-	-	0/1/1/1	-
3	EDO	B	607	-	-	1/1/1/1	-
3	EDO	B	601	-	-	1/1/1/1	-
3	EDO	A	604	-	-	1/1/1/1	-
3	EDO	B	604	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	MES	C8-S	-6.15	1.69	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	608	MES	C5-N4-C3	5.32	120.31	108.84
4	A	608	MES	O3S-S-C8	2.97	111.82	106.00
4	A	608	MES	C7-N4-C5	2.62	118.22	111.24
4	A	608	MES	C7-N4-C3	2.61	118.20	111.24
4	A	608	MES	C8-C7-N4	-2.04	104.63	112.36

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	608	MES	C8-C7-N4-C5
4	A	608	MES	C7-C8-S-O1S
4	A	608	MES	C7-C8-S-O2S
4	A	608	MES	C7-C8-S-O3S
3	B	606	EDO	O1-C1-C2-O2
3	D	602	EDO	O1-C1-C2-O2
4	A	608	MES	C8-C7-N4-C3
3	A	609	EDO	O1-C1-C2-O2
3	B	610	EDO	O1-C1-C2-O2
3	D	604	EDO	O1-C1-C2-O2
3	A	604	EDO	O1-C1-C2-O2
3	B	601	EDO	O1-C1-C2-O2
3	B	608	EDO	O1-C1-C2-O2
3	B	612	EDO	O1-C1-C2-O2
3	F	202	EDO	O1-C1-C2-O2
3	H	201	EDO	O1-C1-C2-O2
3	B	613	EDO	O1-C1-C2-O2
3	G	201	EDO	O1-C1-C2-O2
3	A	605	EDO	O1-C1-C2-O2
3	B	607	EDO	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	201	EDO	1	0
3	B	606	EDO	4	0
3	D	602	EDO	3	0
3	H	201	EDO	1	0
3	A	603	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	609	EDO	2	0
3	B	613	EDO	1	0
3	F	202	EDO	1	0
3	F	201	EDO	1	0
3	B	609	EDO	1	0
3	C	601	EDO	1	0
3	B	610	EDO	2	0
3	C	604	EDO	2	0
3	A	604	EDO	2	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	308/317 (97%)	-0.04	5 (1%) 70 74	10, 19, 31, 41	2 (0%)
1	B	308/317 (97%)	0.13	12 (3%) 43 45	10, 20, 34, 67	3 (0%)
1	C	308/317 (97%)	0.46	16 (5%) 33 33	18, 26, 43, 58	0
1	D	306/317 (96%)	1.24	51 (16%) 4 3	23, 34, 50, 66	0
2	E	126/131 (96%)	0.69	9 (7%) 22 22	17, 27, 43, 66	0
2	F	125/131 (95%)	0.61	8 (6%) 25 26	17, 27, 41, 51	0
2	G	131/131 (100%)	1.11	26 (19%) 3 2	17, 34, 56, 69	1 (0%)
2	H	124/131 (94%)	1.21	16 (12%) 7 7	24, 34, 47, 57	0
All	All	1736/1792 (96%)	0.58	143 (8%) 17 17	10, 27, 46, 69	6 (0%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	42	GLY	5.5
1	B	530	GLY	5.1
1	B	523	PHE	4.4
1	D	524	PHE	4.4
1	D	352	TYR	4.3
2	F	40	ALA	4.1
1	B	411	ASN	4.1
2	F	1	GLN	4.0
1	A	294	THR	3.8
2	G	40	ALA	3.8
1	D	257	PHE	3.8
1	D	258	VAL	3.8
2	E	126	HIS	3.7
2	F	42	GLY	3.7
1	D	412	ASN	3.7
1	C	224	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	294	THR	3.6
2	G	126	HIS	3.6
1	C	294	THR	3.6
1	C	256	ALA	3.6
2	F	125	SER	3.6
2	H	124	SER	3.6
2	F	2	VAL	3.6
2	G	11	LEU	3.5
1	B	521	ASN	3.5
1	D	414	HIS	3.5
1	B	522	GLN	3.4
1	D	523	GLN	3.4
2	F	41	PRO	3.4
1	C	394	THR	3.3
1	B	410	ARG	3.3
1	C	531	GLY	3.2
1	D	426	PHE	3.2
2	H	96	CYS	3.1
1	C	393	GLY	3.1
1	D	252	GLY	3.1
2	H	49	LEU	3.1
1	C	524	PHE	3.0
2	H	66	GLY	3.0
2	H	83	ILE	3.0
2	G	41	PRO	3.0
1	C	340	THR	2.9
1	D	255	SER	2.9
2	G	12	VAL	2.9
1	A	531	GLY	2.8
1	D	418	LEU	2.8
1	D	317	ILE	2.8
1	A	295	GLY	2.8
1	D	293	ILE	2.7
2	H	61	ILE	2.7
1	D	413	THR	2.7
2	G	124	SER	2.7
2	G	2	VAL	2.7
1	D	354	GLY	2.7
1	D	296	SER	2.7
1	D	526	THR	2.7
2	G	14	PRO	2.6
2	G	127	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	255	SER	2.6
2	G	75	ALA	2.6
2	E	124	SER	2.6
1	C	295	GLY	2.6
1	D	259	VAL	2.6
1	D	362	LEU	2.6
2	G	74	ASN	2.6
2	G	84	ASN	2.6
1	D	295	GLY	2.5
2	G	10	GLY	2.5
2	G	86	LEU	2.5
1	B	352[A]	TYR	2.5
1	D	427	PRO	2.5
2	H	108	ARG	2.5
1	D	444	TYR	2.5
1	C	293	ILE	2.5
1	D	527	LEU	2.5
1	D	311	TYR	2.5
1	D	500	ALA	2.5
2	H	42	GLY	2.5
1	D	392	GLY	2.4
1	A	224	THR	2.4
1	D	425	THR	2.4
1	D	485	VAL	2.4
2	G	83	ILE	2.4
1	D	393	GLY	2.4
2	G	125	SER	2.4
1	B	424	THR	2.4
1	D	389	ILE	2.4
1	D	499	VAL	2.4
2	G	123	VAL	2.4
1	D	411	ARG	2.4
1	C	377	ALA	2.4
1	D	422	VAL	2.4
2	E	125	SER	2.3
2	H	29	LEU	2.3
1	C	378	ASN	2.3
1	B	256	ALA	2.3
1	D	405	LEU	2.3
1	D	431	LEU	2.3
2	F	27	PHE	2.3
2	E	74	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	17	SER	2.3
1	C	392	GLY	2.3
2	E	10	GLY	2.3
2	G	131	HIS	2.3
1	A	306	GLN	2.3
1	D	306	GLN	2.3
2	H	1	GLN	2.2
1	B	517	ASP	2.2
1	D	428	GLY	2.2
2	G	60	PHE	2.2
2	G	63	SER	2.2
2	E	11	LEU	2.2
2	E	42	GLY	2.2
2	F	74	ASN	2.2
1	D	521	VAL	2.1
2	G	13	GLN	2.1
1	D	528	ALA	2.1
1	D	410	GLY	2.1
2	G	9	GLY	2.1
1	D	353	THR	2.1
2	E	1	GLN	2.1
2	H	3	GLN	2.1
1	D	403	TRP	2.1
2	G	85	SER	2.1
1	D	367	PHE	2.1
1	D	440	GLY	2.1
2	H	75	ALA	2.1
1	B	520	VAL	2.1
1	D	416	VAL	2.1
1	C	391	ASP	2.1
2	G	16	ASP	2.1
1	B	483	ARG	2.1
1	C	291	THR	2.1
2	H	27	PHE	2.1
2	G	61	ILE	2.1
2	E	75	ALA	2.0
2	H	31	ARG	2.0
1	D	291	THR	2.0
1	D	398	ASN	2.0
1	D	256	ALA	2.0
1	D	419	ALA	2.0
1	D	421	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	64	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
3	EDO	F	202	4/4	0.68	0.18	37,42,43,44	0
3	EDO	B	606	4/4	0.69	0.19	30,30,36,36	0
3	EDO	F	203	4/4	0.79	0.17	35,38,48,56	0
3	EDO	B	612	4/4	0.81	0.12	30,36,41,43	0
3	EDO	B	613	4/4	0.82	0.12	35,42,43,43	0
3	EDO	B	609	4/4	0.82	0.14	33,36,37,42	0
3	EDO	A	604	4/4	0.82	0.16	28,31,32,33	0
3	EDO	F	201	4/4	0.83	0.15	33,35,40,42	0
3	EDO	H	201	4/4	0.84	0.15	41,42,51,54	0
3	EDO	C	602	4/4	0.85	0.13	36,38,41,45	0
3	EDO	E	201	4/4	0.85	0.11	32,39,46,47	0
3	EDO	A	603	4/4	0.86	0.13	31,32,35,44	0
3	EDO	C	605	4/4	0.87	0.12	33,39,47,50	0
3	EDO	D	602	4/4	0.88	0.12	35,36,41,41	0
3	EDO	A	609	4/4	0.89	0.19	20,31,38,38	0
3	EDO	B	601	4/4	0.89	0.13	30,31,36,42	0
3	EDO	A	607	4/4	0.90	0.11	27,31,31,45	0
3	EDO	B	607	4/4	0.90	0.15	27,31,32,34	0
3	EDO	C	604	4/4	0.90	0.12	40,43,47,52	0
3	EDO	A	606	4/4	0.91	0.11	27,31,32,36	0
3	EDO	G	201	4/4	0.91	0.10	35,35,39,40	0
3	EDO	B	608	4/4	0.91	0.19	21,28,30,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MES	A	608	12/12	0.91	0.16	28,44,52,53	0
3	EDO	B	602	4/4	0.92	0.09	23,26,29,30	0
3	EDO	D	603	4/4	0.92	0.11	31,32,39,40	0
3	EDO	B	610	4/4	0.92	0.12	27,32,35,35	0
3	EDO	B	611	4/4	0.92	0.15	22,32,39,41	0
3	EDO	D	601	4/4	0.92	0.11	27,28,31,36	0
3	EDO	A	605	4/4	0.93	0.10	20,24,29,36	0
3	EDO	C	601	4/4	0.93	0.14	26,28,31,34	0
3	EDO	D	604	4/4	0.93	0.10	28,30,35,41	0
3	EDO	B	604	4/4	0.94	0.11	20,22,30,37	0
3	EDO	B	603	4/4	0.94	0.09	21,26,27,30	0
3	EDO	C	603	4/4	0.95	0.09	31,32,33,35	0
3	EDO	A	601	4/4	0.96	0.08	21,21,27,27	0
3	EDO	A	602	4/4	0.96	0.07	21,23,29,31	0
3	EDO	B	605	4/4	0.97	0.08	21,24,28,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.