



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:05 AM UTC

PDB ID : 7TGN / pdb_00007tgn
Title : Crystal structure of DesD, the desferrioxamine synthetase from the Streptomyces violaceus salmycin biosynthetic pathway
Authors : Patel, K.D.; Gulick, A.M.
Deposited on : 2022-01-07
Resolution : 2.30 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

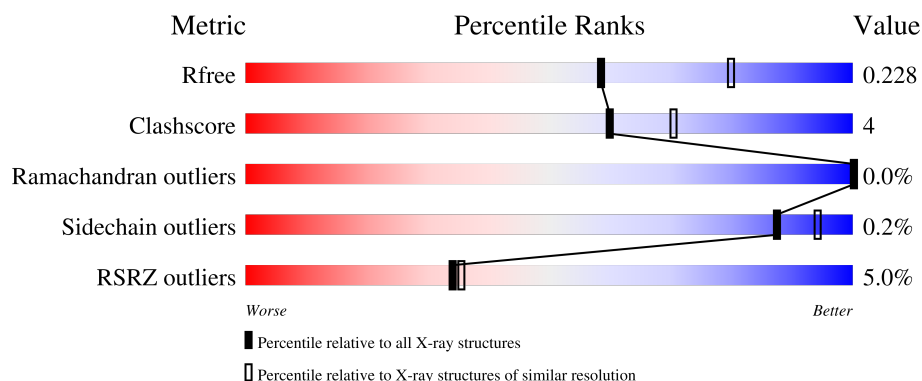
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	609	4% 86% 9% 6%
1	B	609	5% 84% 10% 5%
1	C	609	8% 84% 9% 7%
1	D	609	3% 85% 9% 6%

2 Entry composition [i](#)

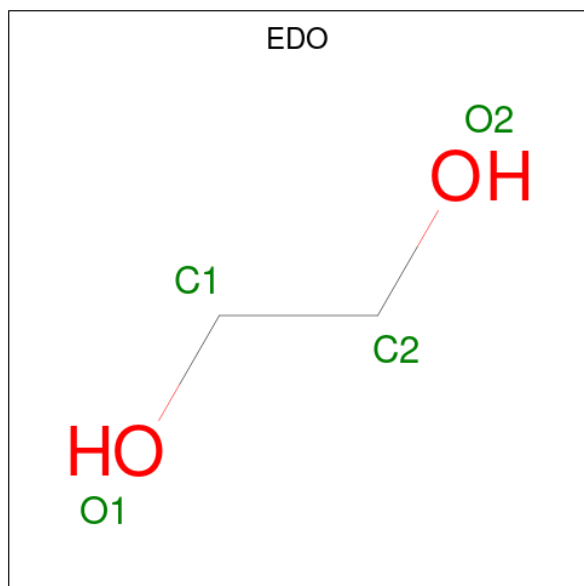
There are 5 unique types of molecules in this entry. The entry contains 17987 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Desferrioxamine synthetase DesD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	0	0
			4408	2827	748	820	13			
1	B	576	Total	C	N	O	S	0	0	0
			4474	2859	770	829	16			
1	C	568	Total	C	N	O	S	0	1	0
			4285	2752	731	787	15			
1	D	570	Total	C	N	O	S	0	1	0
			4464	2854	766	829	15			

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



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

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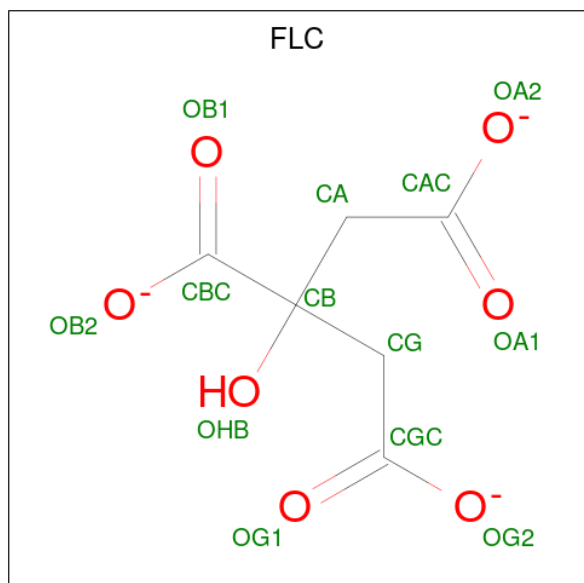
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		

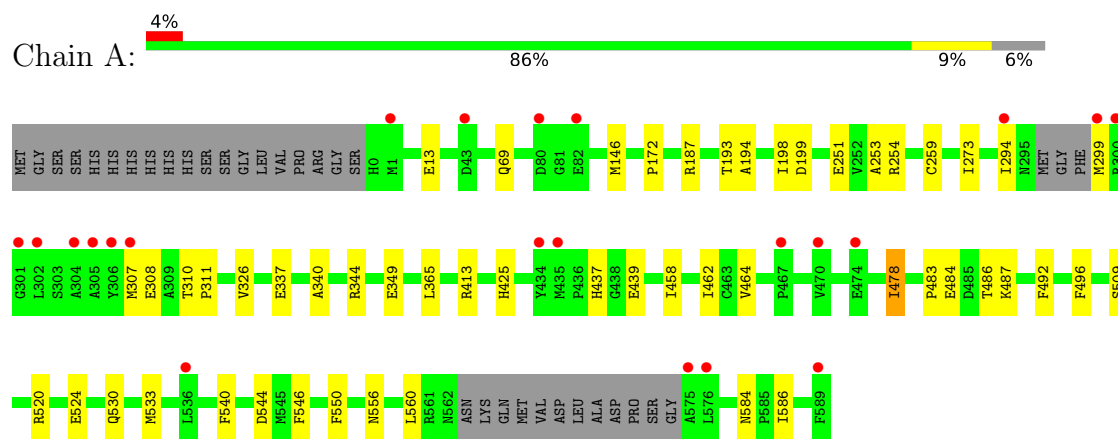
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		
5	B	44	Total	O	0	0
			44	44		
5	C	51	Total	O	0	0
			51	51		
5	D	105	Total	O	0	0
			105	105		

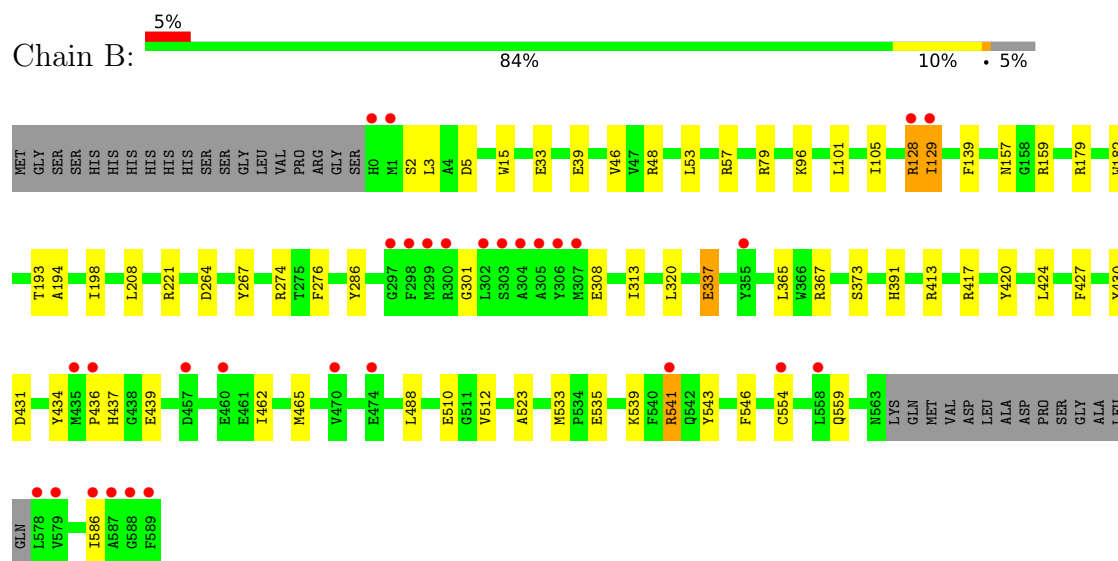
3 Residue-property plots

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.

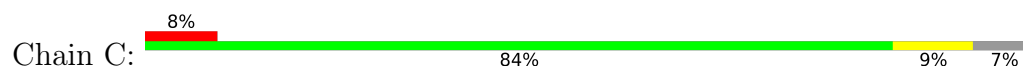
• Molecule 1: Desferrioxamine synthetase DesD

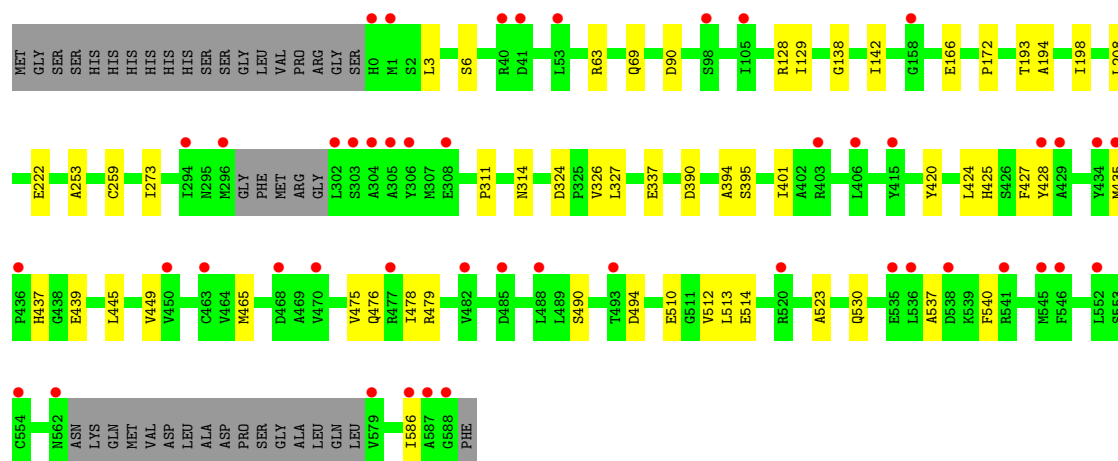


• Molecule 1: Desferrioxamine synthetase DesD

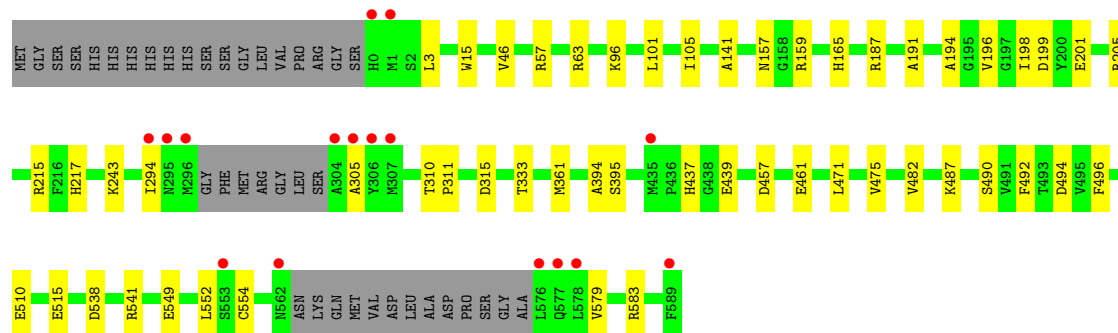
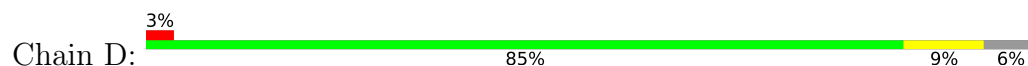


• Molecule 1: Desferrioxamine synthetase DesD





● Molecule 1: Desferrioxamine synthetase DesD



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.53Å 108.53Å 517.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 2.30 49.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.47-2.30) 93.9 (49.47-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.81 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.196 , 0.230 0.197 , 0.228	Depositor DCC
R_{free} test set	2000 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.0	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	17987	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: FLC, MG, EDO

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	0.36	0/4519	0.52	0/6168
1	B	0.41	3/4585 (0.1%)	0.58	3/6247 (0.0%)
1	C	0.36	0/4397	0.55	0/6012
1	D	0.43	0/4577	0.60	0/6234
All	All	0.39	3/18078 (0.0%)	0.57	3/24661 (0.0%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	ILE	CG1-CD1	6.94	1.78	1.51
1	B	541	ARG	CD-NE	-5.32	1.38	1.46
1	B	128	ARG	C-N	5.09	1.40	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	541	ARG	CG-CD-NE	-10.48	88.94	112.00
1	B	541	ARG	CA-CB-CG	-10.40	93.29	114.10
1	B	129	ILE	N-CA-C	5.86	117.59	109.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	541	ARG	Sidechain

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	4408	0	4181	33	0
1	B	4474	0	4295	43	0
1	C	4285	0	4021	40	0
1	D	4464	0	4300	34	0
2	A	16	0	24	3	0
2	B	20	0	30	2	0
2	C	16	0	24	2	0
2	D	40	0	60	6	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	B	13	0	5	0	0
5	A	49	0	0	1	0
5	B	44	0	0	1	0
5	C	51	0	0	3	0
5	D	105	0	0	3	0
All	All	17987	0	16940	148	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 (148) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ILE:CD1	1:B:129:ILE:CG1	1.78	1.55
1:C:222:GLU:OE1	5:C:701:HOH:O	1.89	0.90
1:B:179:ARG:NH1	1:B:264:ASP:O	2.10	0.84
1:A:199:ASP:OD1	5:A:701:HOH:O	1.96	0.82
1:D:437:HIS:HD2	1:D:439:GLU:H	1.27	0.79
1:B:46:VAL:HG22	1:B:57:ARG:HG2	1.67	0.76
1:B:559:GLN:NE2	5:B:701:HOH:O	2.18	0.76
1:D:141:ALA:H	2:D:605:EDO:H21	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:HIS:HD2	1:B:439:GLU:H	1.36	0.71
1:C:166:GLU:OE2	2:C:602:EDO:H22	1.91	0.70
1:A:464:VAL:HG23	1:A:478:ILE:HD12	1.75	0.69
1:C:194:ALA:HB1	1:C:198:ILE:HB	1.75	0.67
1:B:194:ALA:HB1	1:B:198:ILE:HB	1.77	0.67
1:D:215:ARG:NH2	5:D:703:HOH:O	2.27	0.66
1:B:221:ARG:HG3	1:B:221:ARG:HH11	1.61	0.66
1:D:552:LEU:HD23	1:D:579:VAL:HG22	1.78	0.66
1:C:208:LEU:HD23	2:C:604:EDO:H11	1.77	0.65
1:D:199:ASP:OD1	5:D:701:HOH:O	2.15	0.64
1:C:90:ASP:OD1	5:C:702:HOH:O	2.15	0.63
1:C:63:ARG:NH1	1:C:69:GLN:OE1	2.31	0.63
1:A:187:ARG:HH11	2:A:601:EDO:H22	1.64	0.62
1:C:326:VAL:HG21	1:C:425:HIS:ND1	2.15	0.61
1:A:294:ILE:HD13	1:A:299:MET:N	2.16	0.60
1:B:139:PHE:H	2:B:602:EDO:H22	1.67	0.59
1:D:187:ARG:HH11	2:D:603:EDO:H12	1.67	0.59
1:D:457:ASP:O	1:D:461:GLU:HG2	2.03	0.59
1:B:437:HIS:CD2	1:B:439:GLU:H	2.19	0.58
1:B:128:ARG:O	1:B:391:HIS:NE2	2.37	0.58
1:D:437:HIS:CD2	1:D:439:GLU:H	2.17	0.58
1:B:129:ILE:CD1	1:B:129:ILE:CB	2.75	0.58
1:A:69:GLN:NE2	1:A:509:SER:OG	2.35	0.58
1:C:427:PHE:CE1	1:C:465:MET:HE1	2.40	0.56
1:C:476:GLN:HE21	1:C:479:ARG:NH2	2.03	0.56
1:D:165:HIS:HD2	2:D:610:EDO:H11	1.71	0.56
1:A:172:PRO:HD3	1:A:273:ILE:HG22	1.87	0.56
1:C:63:ARG:HH11	1:C:63:ARG:HG3	1.70	0.55
1:C:259:CYS:SG	1:D:3:LEU:HG	2.47	0.55
1:D:538:ASP:OD1	1:D:541:ARG:NH2	2.40	0.55
1:C:437:HIS:HD2	1:C:439:GLU:H	1.54	0.55
1:D:490:SER:O	1:D:494:ASP:HB2	2.07	0.54
1:C:128:ARG:O	1:C:129:ILE:HD13	2.09	0.53
1:B:523:ALA:HB2	1:B:586:ILE:HG23	1.90	0.52
1:A:326:VAL:HB	1:A:425:HIS:CE1	2.44	0.52
1:A:556:ASN:O	1:A:560:LEU:HG	2.09	0.52
1:A:251:GLU:OE2	1:A:254:ARG:NH2	2.43	0.51
1:D:201:GLU:O	1:D:205:ARG:HG3	2.10	0.51
1:C:326:VAL:HG21	1:C:425:HIS:CE1	2.46	0.51
1:B:337:GLU:HG2	1:B:365:LEU:HD13	1.92	0.51
1:D:333:THR:HA	2:D:608:EDO:H22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ARG:O	1:A:524:GLU:HG3	2.12	0.50
1:C:138:GLY:O	1:C:142:ILE:HD12	2.12	0.50
1:A:193:THR:HG21	1:A:308:GLU:O	2.10	0.50
1:A:544:ASP:OD2	1:A:546:PHE:N	2.45	0.49
1:B:101:LEU:HD23	1:B:105:ILE:HD11	1.93	0.49
1:C:3:LEU:O	1:C:6:SER:OG	2.27	0.49
1:D:395:SER:N	1:D:510:GLU:OE2	2.45	0.49
1:B:320:LEU:HD11	1:B:430:TYR:CE1	2.48	0.48
1:D:46:VAL:HG22	1:D:57:ARG:HG2	1.95	0.48
1:A:484:GLU:HA	1:A:487:LYS:HD2	1.96	0.48
1:B:182:TRP:CZ2	1:B:208:LEU:HD21	2.48	0.48
1:B:413:ARG:O	1:B:417:ARG:HG3	2.14	0.48
1:A:492:PHE:O	1:A:496:PHE:HB2	2.14	0.47
1:C:510:GLU:HB3	1:C:512:VAL:HG23	1.95	0.47
1:D:196:VAL:HG23	1:D:315:ASP:OD2	2.14	0.47
1:D:191:ALA:HA	2:D:603:EDO:H21	1.97	0.47
2:D:604:EDO:H22	2:D:610:EDO:H22	1.96	0.47
1:B:391:HIS:H	1:B:391:HIS:CD2	2.30	0.47
1:B:510:GLU:HB3	1:B:512:VAL:HG23	1.96	0.47
1:C:523:ALA:HB2	1:C:586:ILE:HG23	1.96	0.47
1:A:259:CYS:SG	1:B:3:LEU:HG	2.55	0.47
1:B:128:ARG:O	1:B:391:HIS:CD2	2.68	0.46
1:B:286:TYR:HB2	1:B:367:ARG:HB3	1.97	0.46
1:C:530:GLN:HG2	1:C:540:PHE:CE2	2.50	0.46
1:D:471:LEU:HD13	1:D:475:VAL:HG12	1.97	0.46
1:D:482:VAL:CG2	1:D:487:LYS:HG2	2.45	0.46
1:A:413:ARG:NH1	1:A:524:GLU:OE2	2.48	0.46
1:B:157:ASN:O	1:B:159:ARG:HD2	2.15	0.46
1:D:243:LYS:HB3	1:D:361:MET:CE	2.46	0.46
1:A:13:GLU:H	1:A:13:GLU:CD	2.24	0.46
1:A:344:ARG:HD2	1:A:349:GLU:OE2	2.15	0.46
1:C:490:SER:O	1:C:494:ASP:HB2	2.15	0.46
1:B:313:ILE:CG2	1:B:462:ILE:HD11	2.46	0.46
1:C:537:ALA:HA	1:C:540:PHE:CD2	2.51	0.46
1:C:427:PHE:HE1	1:C:465:MET:HE1	1.81	0.46
1:B:535:GLU:H	1:B:535:GLU:CD	2.24	0.46
1:A:483:PRO:HB2	1:A:486:THR:HG23	1.98	0.46
1:C:324:ASP:OD1	1:C:326:VAL:HG22	2.16	0.46
1:D:157:ASN:O	1:D:159:ARG:HD2	2.15	0.46
1:C:314:ASN:ND2	1:C:337:GLU:HB2	2.31	0.45
1:A:533:MET:HE3	1:A:533:MET:HB3	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LYS:NZ	1:B:101:LEU:O	2.49	0.45
1:B:33:GLU:OE1	1:B:554:CYS:HB3	2.16	0.45
1:B:267:TYR:HB3	1:B:276:PHE:HB3	1.99	0.45
1:C:513:LEU:HD23	1:C:514:GLU:O	2.16	0.45
1:D:194:ALA:HB1	1:D:198:ILE:HB	1.99	0.45
2:A:601:EDO:H12	5:C:723:HOH:O	2.17	0.45
1:C:476:GLN:HG2	1:C:479:ARG:CZ	2.47	0.45
1:D:492:PHE:O	1:D:496:PHE:HB2	2.17	0.45
1:B:39:GLU:OE1	1:B:48:ARG:NH2	2.50	0.44
1:C:193:THR:HG22	1:C:311:PRO:HG2	1.99	0.44
1:C:435:MET:HE2	1:C:435:MET:HB3	1.77	0.44
1:C:445:LEU:HA	1:C:449:VAL:O	2.17	0.44
1:D:63:ARG:HD2	1:D:515:GLU:OE2	2.17	0.44
1:D:294:ILE:HD12	1:D:294:ILE:N	2.33	0.44
1:B:431:ASP:OD1	1:B:539:LYS:NZ	2.50	0.44
1:C:63:ARG:NH1	1:C:63:ARG:HG3	2.32	0.44
1:A:310:THR:HB	1:A:311:PRO:HD3	2.00	0.44
1:C:395:SER:HB3	1:C:510:GLU:OE2	2.18	0.44
1:C:420:TYR:CE2	1:C:424:LEU:HD11	2.53	0.44
1:A:464:VAL:HG23	1:A:478:ILE:CD1	2.43	0.44
1:B:2:SER:HB3	1:B:5:ASP:OD2	2.18	0.43
1:B:53:LEU:O	1:B:79:ARG:HG3	2.18	0.43
1:D:96:LYS:NZ	1:D:101:LEU:O	2.49	0.43
1:A:530:GLN:HA	1:A:540:PHE:CE1	2.53	0.43
1:B:274:ARG:NH1	1:B:301:GLY:O	2.52	0.43
1:C:172:PRO:HD3	1:C:273:ILE:HG22	1.99	0.43
1:D:554:CYS:SG	1:D:579:VAL:HG11	2.59	0.43
1:A:492:PHE:HB3	1:A:550:PHE:CE1	2.54	0.43
1:A:146:MET:HA	1:A:146:MET:HE2	2.01	0.42
1:B:193:THR:HG21	1:B:308:GLU:O	2.20	0.42
1:B:533:MET:HE3	1:B:533:MET:HB3	1.81	0.42
1:C:475:VAL:O	1:C:478:ILE:HG12	2.20	0.42
1:A:337:GLU:HG2	1:A:365:LEU:HD13	2.01	0.42
1:B:427:PHE:CE1	1:B:465:MET:HE1	2.55	0.42
1:D:549:GLU:HG2	1:D:583:ARG:HA	2.01	0.42
1:D:394:ALA:HA	1:D:510:GLU:OE2	2.19	0.42
1:A:187:ARG:HG2	2:A:601:EDO:H11	2.02	0.42
1:A:584:ASN:OD1	1:A:586:ILE:HG12	2.20	0.42
1:B:488:LEU:HD22	1:B:543:TYR:HB3	2.02	0.42
1:B:546:PHE:CE2	1:B:586:ILE:HG21	2.55	0.42
1:A:458:ILE:O	1:A:462:ILE:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:530:GLN:HG2	1:C:540:PHE:CZ	2.54	0.41
1:A:253:ALA:HB1	1:B:15:TRP:HB2	2.02	0.41
1:D:310:THR:HB	1:D:311:PRO:HD3	2.01	0.41
1:A:307:MET:CG	1:A:340:ALA:HB1	2.50	0.41
1:B:434:TYR:C	1:B:436:PRO:HD3	2.45	0.41
1:C:428:TYR:CD1	1:C:540:PHE:HE1	2.38	0.41
1:A:194:ALA:HB1	1:A:198:ILE:HB	2.01	0.41
1:B:373:SER:HB3	2:B:604:EDO:H21	2.02	0.41
1:C:327:LEU:HD23	1:C:327:LEU:HA	1.87	0.41
1:C:390:ASP:OD2	1:C:394:ALA:HB3	2.20	0.41
1:C:465:MET:HB2	1:C:465:MET:HE3	1.60	0.41
1:B:221:ARG:HG3	1:B:221:ARG:NH1	2.33	0.41
1:D:217:HIS:HE1	5:D:797:HOH:O	2.04	0.41
1:C:253:ALA:HB1	1:D:15:TRP:HB2	2.04	0.40
1:A:437:HIS:NE2	1:A:439:GLU:HB2	2.36	0.40
1:D:105:ILE:H	1:D:105:ILE:HG13	1.77	0.40
1:B:420:TYR:CE2	1:B:424:LEU:HD11	2.57	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	569/609 (93%)	554 (97%)	15 (3%)	0	100	100
1	B	572/609 (94%)	550 (96%)	22 (4%)	0	100	100
1	C	563/609 (92%)	544 (97%)	19 (3%)	0	100	100
1	D	565/609 (93%)	550 (97%)	14 (2%)	1 (0%)	43	55
All	All	2269/2436 (93%)	2198 (97%)	70 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	305	ALA

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	437/506 (86%)	436 (100%)	1 (0%)	87	94
1	B	452/506 (89%)	451 (100%)	1 (0%)	87	94
1	C	414/506 (82%)	413 (100%)	1 (0%)	87	94
1	D	455/506 (90%)	455 (100%)	0	100	100
All	All	1758/2024 (87%)	1755 (100%)	3 (0%)	87	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	478	ILE
1	B	337	GLU
1	C	401	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	256	HIS
1	A	270	GLN
1	A	271	GLN
1	A	425	HIS
1	B	140	GLN
1	B	256	HIS
1	B	270	GLN
1	B	391	HIS
1	B	437	HIS
1	C	157	ASN
1	C	242	ASN
1	C	271	GLN

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Mol	Chain	Res	Type
1	C	281	HIS
1	C	388	HIS
1	C	437	HIS
1	C	476	GLN
1	C	530	GLN
1	D	437	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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	$\# Z > 2$
2	EDO	B	601	-	3,3,3	0.52	0	2,2,2	0.27	0
2	EDO	D	601	-	3,3,3	0.65	0	2,2,2	0.80	0
2	EDO	A	603	-	3,3,3	0.44	0	2,2,2	0.45	0
2	EDO	A	601	-	3,3,3	0.43	0	2,2,2	1.00	0
2	EDO	B	604	-	3,3,3	0.54	0	2,2,2	0.24	0
2	EDO	B	605	-	3,3,3	0.55	0	2,2,2	0.27	0
2	EDO	D	606	-	3,3,3	0.70	0	2,2,2	0.22	0
2	EDO	B	602	-	3,3,3	0.28	0	2,2,2	1.64	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	D	607	-	3,3,3	0.61	0	2,2,2	0.24	0
2	EDO	C	603	-	3,3,3	0.44	0	2,2,2	0.74	0
2	EDO	A	604	-	3,3,3	0.44	0	2,2,2	0.32	0
2	EDO	D	604	-	3,3,3	0.39	0	2,2,2	0.52	0
2	EDO	D	603	-	3,3,3	0.86	0	2,2,2	0.80	0
2	EDO	D	602	-	3,3,3	0.28	0	2,2,2	1.65	0
2	EDO	C	601	-	3,3,3	0.27	0	2,2,2	0.68	0
2	EDO	D	605	-	3,3,3	0.69	0	2,2,2	0.39	0
2	EDO	C	602	-	3,3,3	0.50	0	2,2,2	0.52	0
2	EDO	C	604	-	3,3,3	0.72	0	2,2,2	0.10	0
2	EDO	A	602	-	3,3,3	0.90	0	2,2,2	0.10	0
2	EDO	B	603	-	3,3,3	0.61	0	2,2,2	0.17	0
2	EDO	D	609	-	3,3,3	0.56	0	2,2,2	0.07	0
2	EDO	D	610	-	3,3,3	0.45	0	2,2,2	0.44	0
4	FLC	B	606	-	12,12,12	1.13	2 (16%)	17,17,17	1.05	2 (11%)
2	EDO	D	608	-	3,3,3	0.48	0	2,2,2	0.18	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
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	D	601	-	-	1/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	B	604	-	-	0/1/1/1	-
2	EDO	B	605	-	-	0/1/1/1	-
2	EDO	D	606	-	-	1/1/1/1	-
2	EDO	B	602	-	-	0/1/1/1	-
2	EDO	D	607	-	-	0/1/1/1	-
2	EDO	C	603	-	-	1/1/1/1	-
2	EDO	A	604	-	-	0/1/1/1	-
2	EDO	D	604	-	-	0/1/1/1	-
2	EDO	D	603	-	-	1/1/1/1	-
2	EDO	D	602	-	-	1/1/1/1	-
2	EDO	C	601	-	-	0/1/1/1	-
2	EDO	D	605	-	-	1/1/1/1	-
2	EDO	C	602	-	-	0/1/1/1	-
2	EDO	C	604	-	-	1/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	603	-	-	1/1/1/1	-
2	EDO	D	609	-	-	0/1/1/1	-
2	EDO	D	610	-	-	0/1/1/1	-
4	FLC	B	606	-	-	2/16/16/16	-
2	EDO	D	608	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	606	FLC	OG1-CGC	2.94	1.31	1.22
4	B	606	FLC	OG2-CGC	-2.40	1.22	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	606	FLC	OG1-CGC-CG	-3.27	113.68	122.95
4	B	606	FLC	OG2-CGC-CG	2.77	123.12	114.35
2	B	602	EDO	O2-C2-C1	-2.15	96.03	112.39

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	EDO	O1-C1-C2-O2
2	D	603	EDO	O1-C1-C2-O2
2	A	602	EDO	O1-C1-C2-O2
2	B	603	EDO	O1-C1-C2-O2
2	D	605	EDO	O1-C1-C2-O2
2	D	606	EDO	O1-C1-C2-O2
2	C	604	EDO	O1-C1-C2-O2
4	B	606	FLC	CB-CG-CGC-OG1
2	C	603	EDO	O1-C1-C2-O2
2	D	602	EDO	O1-C1-C2-O2
4	B	606	FLC	CB-CG-CGC-OG2

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	604	EDO	1	0
2	B	602	EDO	1	0
2	D	604	EDO	1	0
2	D	603	EDO	2	0
2	D	605	EDO	1	0
2	C	602	EDO	1	0
2	C	604	EDO	1	0
2	D	610	EDO	2	0
2	D	608	EDO	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	575/609 (94%)	0.32	22 (3%)	44	46	42, 71, 105, 132	0
1	B	576/609 (94%)	0.29	30 (5%)	33	34	48, 67, 99, 133	0
1	C	568/609 (93%)	0.58	47 (8%)	17	19	36, 81, 121, 143	1 (0%)
1	D	570/609 (93%)	0.00	16 (2%)	55	57	36, 54, 84, 127	1 (0%)
All	All	2289/2436 (93%)	0.30	115 (5%)	34	35	36, 66, 110, 143	2 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	306	TYR	6.4
1	A	299	MET	5.8
1	C	294	ILE	5.7
1	B	306	TYR	5.6
1	D	305	ALA	5.4
1	C	306	TYR	5.0
1	C	296	MET	4.8
1	D	295	ASN	4.5
1	D	304	ALA	4.5
1	B	589	PHE	4.4
1	B	586	ILE	4.1
1	A	294	ILE	4.1
1	A	300	ARG	3.9
1	C	586	ILE	3.9
1	C	1	MET	3.8
1	B	579	VAL	3.8
1	D	0	HIS	3.8
1	C	588	GLY	3.7
1	C	304	ALA	3.6
1	D	577	GLN	3.6
1	B	578	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	587	ALA	3.6
1	D	1	MET	3.5
1	A	306	TYR	3.4
1	B	298	PHE	3.4
1	A	575	ALA	3.4
1	A	1	MET	3.4
1	C	305	ALA	3.3
1	B	299	MET	3.3
1	D	296	MET	3.3
1	D	576	LEU	3.2
1	A	43	ASP	3.2
1	A	301	GLY	3.1
1	D	294	ILE	3.0
1	D	553	SER	3.0
1	B	0	HIS	3.0
1	B	128	ARG	3.0
1	B	304	ALA	3.0
1	D	578	LEU	3.0
1	C	303	SER	3.0
1	D	562	ASN	2.9
1	C	302	LEU	2.9
1	C	429	ALA	2.8
1	A	435	MET	2.8
1	C	554	CYS	2.8
1	A	304	ALA	2.8
1	B	435	MET	2.8
1	D	589	PHE	2.8
1	C	482	VAL	2.7
1	C	579	VAL	2.7
1	A	307	MET	2.6
1	B	355	TYR	2.6
1	C	434	TYR	2.6
1	A	576	LEU	2.6
1	C	435	MET	2.6
1	C	436	PRO	2.6
1	A	536	LEU	2.6
1	C	403	ARG	2.6
1	C	485	ASP	2.6
1	B	297	GLY	2.6
1	C	0	HIS	2.6
1	C	477	ARG	2.5
1	C	587	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	470	VAL	2.5
1	B	457	ASP	2.5
1	C	538	ASP	2.5
1	C	536	LEU	2.5
1	D	307	MET	2.5
1	C	562	ASN	2.5
1	A	474	GLU	2.5
1	B	300	ARG	2.5
1	C	546	PHE	2.4
1	A	80	ASP	2.4
1	B	541	ARG	2.4
1	B	129	ILE	2.4
1	C	40	ARG	2.4
1	A	305	ALA	2.4
1	B	305	ALA	2.4
1	C	552	LEU	2.4
1	B	303	SER	2.4
1	B	302	LEU	2.4
1	C	428	TYR	2.3
1	B	470	VAL	2.3
1	D	435	MET	2.3
1	A	467	PRO	2.3
1	B	588	GLY	2.3
1	A	82	GLU	2.3
1	C	158	GLY	2.2
1	C	105	ILE	2.2
1	C	406	LEU	2.2
1	B	307	MET	2.2
1	B	554	CYS	2.2
1	C	545	MET	2.2
1	C	535	GLU	2.2
1	C	541	ARG	2.1
1	B	1	MET	2.1
1	B	460	GLU	2.1
1	B	474	GLU	2.1
1	A	434	TYR	2.1
1	C	493	THR	2.1
1	A	302	LEU	2.1
1	C	415	TYR	2.1
1	C	468	ASP	2.1
1	B	436	PRO	2.1
1	C	450	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	470	VAL	2.1
1	C	98	SER	2.1
1	C	53	LEU	2.1
1	C	488	LEU	2.1
1	A	589	PHE	2.1
1	C	41	ASP	2.0
1	C	520	ARG	2.0
1	C	308	GLU	2.0
1	C	463	CYS	2.0
1	B	558	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
2	EDO	C	604	4/4	0.70	0.28	55,60,63,75	0
4	FLC	B	606	13/13	0.72	0.13	100,105,113,121	0
2	EDO	C	601	4/4	0.78	0.26	71,76,78,91	0
2	EDO	D	601	4/4	0.79	0.24	55,57,58,79	0
2	EDO	C	602	4/4	0.79	0.20	57,62,64,68	0
2	EDO	D	609	4/4	0.81	0.16	65,69,72,92	0
2	EDO	D	610	4/4	0.81	0.17	66,70,78,79	0
2	EDO	B	605	4/4	0.81	0.16	64,69,72,84	0
2	EDO	B	603	4/4	0.82	0.20	74,76,80,83	0
2	EDO	D	603	4/4	0.83	0.22	49,59,68,70	0
2	EDO	A	603	4/4	0.84	0.18	67,67,84,86	0
2	EDO	B	604	4/4	0.86	0.13	64,67,67,81	0
2	EDO	B	602	4/4	0.86	0.19	55,60,63,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	D	602	4/4	0.87	0.15	45,48,55,58	0
2	EDO	C	603	4/4	0.87	0.20	67,79,90,94	0
2	EDO	D	605	4/4	0.87	0.17	53,58,68,69	0
2	EDO	D	606	4/4	0.88	0.14	48,56,59,71	0
2	EDO	A	604	4/4	0.88	0.13	63,65,76,79	0
2	EDO	D	608	4/4	0.89	0.15	58,63,68,89	0
2	EDO	A	602	4/4	0.90	0.14	48,56,65,65	0
2	EDO	D	604	4/4	0.90	0.15	63,63,63,84	0
2	EDO	A	601	4/4	0.91	0.15	54,55,59,73	0
2	EDO	B	601	4/4	0.91	0.16	55,55,59,84	0
3	MG	A	605	1/1	0.94	0.07	61,61,61,61	0
3	MG	C	605	1/1	0.95	0.12	54,54,54,54	0
2	EDO	D	607	4/4	0.95	0.10	51,54,56,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.