



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:12 AM UTC

PDB ID : 5U0L / pdb_00005u0l
Title : X-ray crystal structure of fatty aldehyde dehydrogenase enzymes from *Marinobacter aquaeolei* VT8 complexed with a substrate
Authors : Shi, K.; Mulliner, K.; Barney, B.M.; Aihara, H.
Deposited on : 2016-11-24
Resolution : 2.29 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

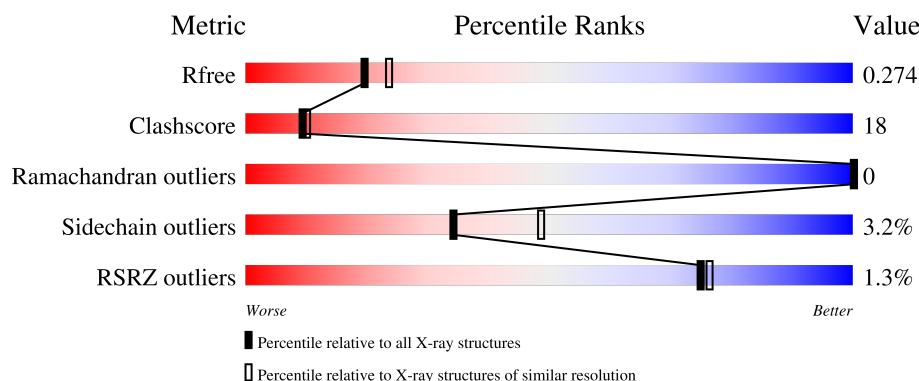
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	497	% 70% 26% ..
1	B	497	% 68% 29% ..

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
4	MPD	B	501	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7537 atoms, of which 65 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 N-succinylglutamate 5-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3679	2328	646	694	11			
1	B	487	Total	C	N	O	S	0	0	0
			3671	2324	644	692	11			

There are 14 discrepancies between the modelled and reference sequences:

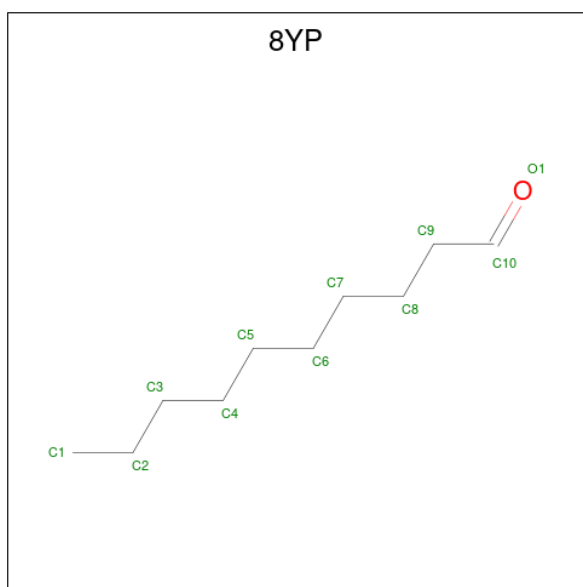
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP A1U5W8
A	-4	HIS	-	expression tag	UNP A1U5W8
A	-3	HIS	-	expression tag	UNP A1U5W8
A	-2	HIS	-	expression tag	UNP A1U5W8
A	-1	HIS	-	expression tag	UNP A1U5W8
A	0	HIS	-	expression tag	UNP A1U5W8
A	1	HIS	-	expression tag	UNP A1U5W8
B	-5	MET	-	initiating methionine	UNP A1U5W8
B	-4	HIS	-	expression tag	UNP A1U5W8
B	-3	HIS	-	expression tag	UNP A1U5W8
B	-2	HIS	-	expression tag	UNP A1U5W8
B	-1	HIS	-	expression tag	UNP A1U5W8
B	0	HIS	-	expression tag	UNP A1U5W8
B	1	HIS	-	expression tag	UNP A1U5W8

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



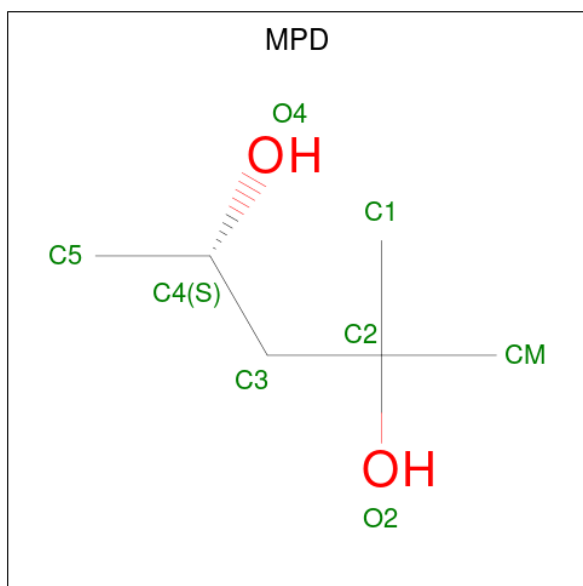
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is decanal (CCD ID: 8YP) (formula: $C_{10}H_{20}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	H	0	0
			25	8	17		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).

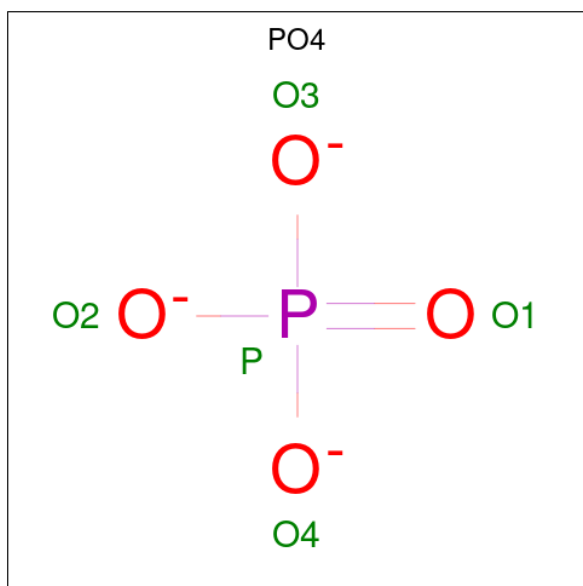


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O P 5 4 1	0	0

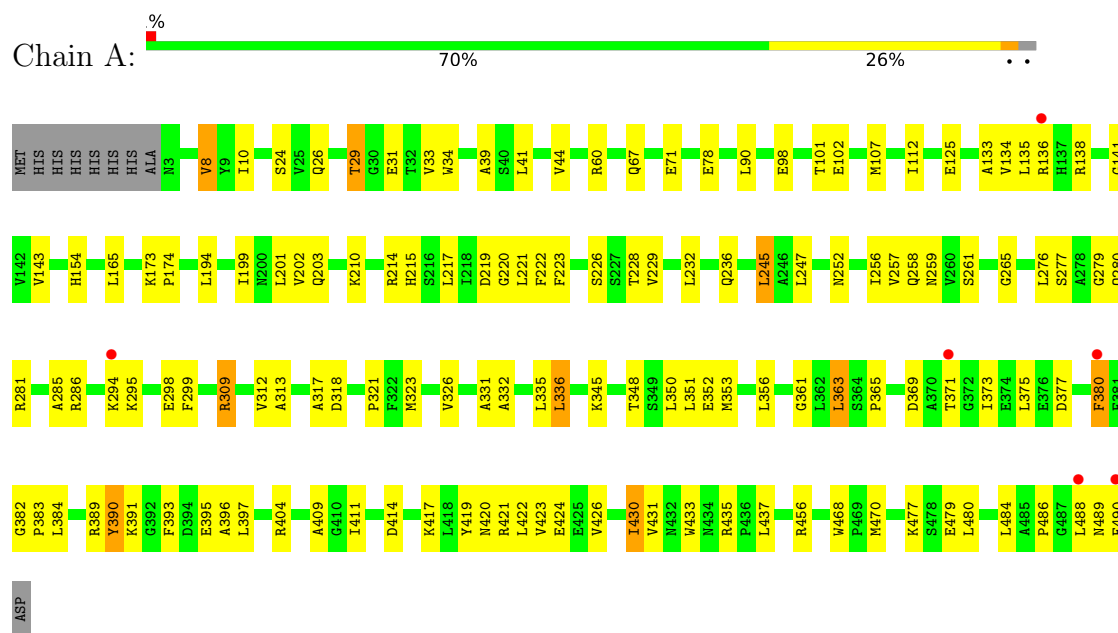
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	39	Total O 39 39	0	0
7	B	21	Total O 21 21	0	0

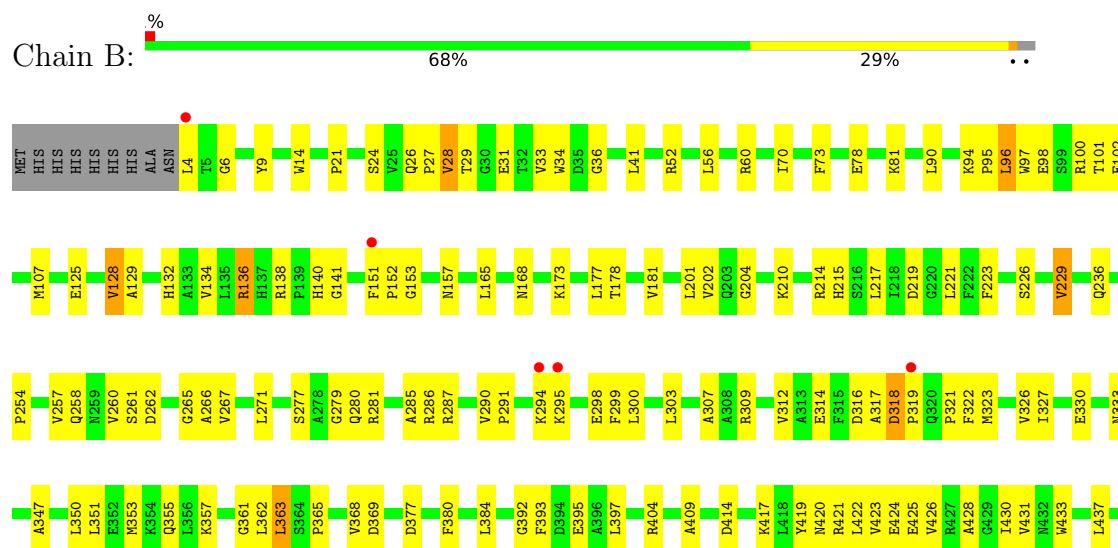
3 Residue-property plots

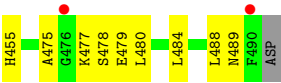
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: N-succinylglutamate 5-semialdehyde dehydrogenase



- Molecule 1: N-succinylglutamate 5-semialdehyde dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.71Å 98.71Å 254.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.90 – 2.29 34.90 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.4 (34.90-2.29) 97.7 (34.90-2.29)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.29Å)	Xtriage
Refinement program	PHENIX dev_2706	Depositor
R, R_{free}	0.214 , 0.270 0.227 , 0.274	Depositor DCC
R_{free} test set	2748 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.3	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	0.96	EDS
Total number of atoms	7537	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% 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: MPD, CL, PO4, EDO, 8YP

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	0.44	0/3761	0.63	0/5110
1	B	0.40	0/3753	0.58	0/5099
All	All	0.42	0/7514	0.60	0/10209

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

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	3679	0	3637	141	0
1	B	3671	0	3631	147	0
2	A	32	48	48	3	0
3	A	8	17	0	0	0
4	B	16	0	28	15	0
5	B	1	0	0	0	0
6	B	5	0	0	0	0
7	A	39	0	0	0	0
7	B	21	0	0	0	0
All	All	7472	65	7344	266	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 18.

All (266) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:MET:HE1	1:B:423:VAL:HG13	1.29	1.11
1:A:39:ALA:CB	1:A:202:VAL:HG13	1.96	0.95
1:B:294:LYS:HG3	1:B:295:LYS:HD3	1.49	0.94
1:A:477:LYS:HD3	1:B:414:ASP:OD1	1.72	0.89
1:B:152:PRO:HB2	1:B:181:VAL:HG11	1.54	0.88
1:B:226:SER:OG	1:B:229:VAL:HG12	1.76	0.85
1:A:226:SER:OG	1:A:229:VAL:HG12	1.77	0.85
1:A:279:GLY:O	1:A:286:ARG:NH2	2.11	0.84
1:A:377:ASP:OD2	1:A:404:ARG:HD3	1.78	0.84
1:B:210:LYS:HD3	1:B:214:ARG:HH22	1.41	0.83
1:A:480:LEU:HD23	1:A:484:LEU:HD21	1.62	0.82
1:B:314:GLU:OE2	1:B:357:LYS:NZ	2.14	0.81
1:B:210:LYS:HB3	1:B:214:ARG:NH2	1.96	0.80
1:B:285:ALA:HB2	1:B:437:LEU:HD12	1.64	0.79
1:A:60:ARG:NH2	1:B:425:GLU:OE1	2.15	0.79
1:A:414:ASP:OD1	1:B:477:LYS:HD3	1.85	0.76
1:A:78:GLU:OE1	1:A:107:MET:HE1	1.86	0.76
1:A:257:VAL:HG11	1:A:299:PHE:CE2	2.21	0.75
1:B:267:VAL:HG13	1:B:303:LEU:HD12	1.68	0.75
1:A:39:ALA:HB3	1:A:202:VAL:HG13	1.66	0.75
1:A:480:LEU:HD11	1:A:490:PHE:HE2	1.52	0.75
1:B:98:GLU:OE2	1:B:277:SER:OG	2.03	0.75
1:A:335:LEU:HD21	1:A:382:GLY:HA3	1.68	0.74
1:A:488:LEU:HD21	1:B:322:PHE:CD1	2.23	0.74
1:A:477:LYS:NZ	1:B:261:SER:OG	2.19	0.73
1:B:290:VAL:HG11	1:B:300:LEU:HD21	1.70	0.73
1:B:29:THR:OG1	1:B:31:GLU:HG2	1.87	0.73
1:B:257:VAL:CG1	1:B:290:VAL:HG22	2.19	0.73
1:B:151:PHE:CZ	1:B:281:ARG:HG2	2.24	0.72
1:A:277:SER:O	1:A:280:GLN:HG3	1.88	0.72
1:B:393:PHE:H	4:B:501:MPD:C3	2.03	0.71
1:A:373:ILE:HG22	1:A:375:LEU:HD12	1.72	0.71
1:A:480:LEU:HD21	1:A:490:PHE:CE2	2.25	0.71
1:A:351:LEU:HD22	1:A:365:PRO:O	1.92	0.70
1:B:377:ASP:OD2	1:B:404:ARG:HD3	1.91	0.69
1:A:390:TYR:CE2	1:A:396:ALA:HB2	2.26	0.69
1:B:151:PHE:HZ	1:B:281:ARG:HG2	1.57	0.69
1:A:29:THR:HG22	1:A:31:GLU:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:SER:H	1:B:477:LYS:HZ1	1.42	0.68
1:B:393:PHE:HB3	4:B:501:MPD:H31	1.75	0.68
1:B:422:LEU:HD12	1:B:426:VAL:HB	1.76	0.68
1:B:477:LYS:HD2	1:B:478:SER:N	2.08	0.68
1:A:280:GLN:NE2	1:A:326:VAL:HA	2.08	0.68
1:B:477:LYS:HD2	1:B:478:SER:H	1.58	0.68
1:A:391:LYS:HB2	1:A:395:GLU:OE1	1.94	0.67
1:B:393:PHE:H	4:B:501:MPD:H32	1.61	0.66
1:B:258:GLN:HE22	4:B:501:MPD:HM2	1.61	0.66
1:A:373:ILE:HG22	1:A:375:LEU:CD1	2.24	0.66
1:A:421:ARG:HH22	2:A:501:EDO:H11	1.61	0.66
1:A:265:GLY:HA2	1:B:480:LEU:HD22	1.77	0.66
1:A:136:ARG:HD3	1:A:136:ARG:N	2.12	0.65
1:A:317:ALA:HB3	1:A:321:PRO:HD3	1.79	0.65
1:B:326:VAL:HG22	1:B:361:GLY:O	1.97	0.65
1:A:135:LEU:C	1:A:136:ARG:HD3	2.22	0.64
1:A:480:LEU:HD12	1:B:265:GLY:HA2	1.79	0.64
1:B:393:PHE:CB	4:B:501:MPD:H31	2.27	0.64
1:B:125:GLU:HG2	1:B:132:HIS:CE1	2.32	0.64
1:B:280:GLN:NE2	1:B:326:VAL:HA	2.12	0.64
1:A:214:ARG:HG2	1:A:236:GLN:NE2	2.12	0.64
1:A:261:SER:N	1:B:477:LYS:HZ1	1.96	0.64
1:A:477:LYS:HE2	1:B:262:ASP:HB3	1.80	0.63
1:B:26:GLN:OE1	1:B:28:VAL:HG13	1.99	0.63
1:A:422:LEU:HD12	1:A:426:VAL:HB	1.80	0.63
4:B:501:MPD:O4	4:B:501:MPD:H12	1.99	0.63
1:B:277:SER:O	1:B:280:GLN:HG3	1.98	0.62
1:B:318:ASP:OD1	1:B:318:ASP:N	2.27	0.62
1:A:44:VAL:HG22	1:A:202:VAL:HG11	1.82	0.62
1:A:252:ASN:HD21	2:A:505:EDO:H22	1.63	0.62
1:B:290:VAL:HG11	1:B:300:LEU:CD2	2.29	0.62
1:B:78:GLU:OE1	1:B:107:MET:HE1	1.99	0.62
1:B:351:LEU:HD22	1:B:365:PRO:O	1.99	0.61
1:B:136:ARG:N	1:B:136:ARG:HD2	2.14	0.61
1:B:152:PRO:CB	1:B:181:VAL:HG11	2.26	0.61
1:A:294:LYS:HG3	1:A:295:LYS:HD3	1.83	0.60
1:A:298:GLU:HG3	1:A:299:PHE:N	2.15	0.60
1:B:152:PRO:HB2	1:B:181:VAL:CG1	2.27	0.60
1:A:435:ARG:CD	1:B:475:ALA:HB2	2.33	0.59
1:B:214:ARG:HG2	1:B:236:GLN:NE2	2.17	0.59
1:B:56:LEU:O	1:B:60:ARG:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HD22	1:A:281:ARG:NE	2.18	0.58
1:B:136:ARG:HD2	1:B:136:ARG:H	1.69	0.58
1:A:380:PHE:C	1:A:380:PHE:HD1	2.11	0.58
1:B:317:ALA:HB3	1:B:321:PRO:HD3	1.86	0.58
1:A:326:VAL:HG22	1:A:361:GLY:O	2.03	0.58
1:A:380:PHE:HD1	1:A:380:PHE:O	1.87	0.57
1:A:335:LEU:CD2	1:A:382:GLY:HA3	2.34	0.57
1:A:489:ASN:HB3	1:B:309:ARG:HD3	1.86	0.57
1:B:271:LEU:HD21	1:B:307:ALA:HB2	1.87	0.57
1:B:417:LYS:HD2	1:B:420:ASN:HB2	1.86	0.56
1:A:215:HIS:CE1	1:A:217:LEU:HB2	2.40	0.56
1:B:214:ARG:HH11	1:B:236:GLN:HE22	1.53	0.56
1:B:350:LEU:HD11	1:B:369:ASP:HB2	1.86	0.56
1:A:380:PHE:C	1:A:380:PHE:CD1	2.83	0.56
1:B:81:LYS:NZ	1:B:100:ARG:O	2.37	0.56
1:B:409:ALA:O	1:B:431:VAL:HA	2.05	0.56
1:A:228:THR:O	1:A:232:LEU:HD22	2.05	0.56
1:A:245:LEU:HD13	1:A:247:LEU:HG	1.88	0.56
1:B:125:GLU:HG2	1:B:132:HIS:NE2	2.21	0.55
1:B:393:PHE:H	4:B:501:MPD:H31	1.69	0.55
1:A:350:LEU:HD11	1:A:369:ASP:HB2	1.87	0.55
1:B:214:ARG:HH11	1:B:236:GLN:NE2	2.04	0.55
1:A:375:LEU:HD12	1:A:375:LEU:N	2.22	0.55
1:A:78:GLU:HB2	1:A:107:MET:CE	2.37	0.55
1:A:456:ARG:NH1	4:B:502:MPD:H53	2.21	0.55
1:B:312:VAL:CG2	1:B:323:MET:HE2	2.38	0.54
1:B:223:PHE:HZ	1:B:229:VAL:HG13	1.73	0.54
1:B:419:TYR:CD1	1:B:433:TRP:HB2	2.43	0.54
1:A:409:ALA:O	1:A:431:VAL:HA	2.06	0.54
1:B:357:LYS:HD2	1:B:362:LEU:HD12	1.88	0.54
1:B:223:PHE:CZ	1:B:229:VAL:HG13	2.41	0.54
1:B:480:LEU:HD12	1:B:484:LEU:HD11	1.88	0.54
1:A:39:ALA:HB2	1:A:202:VAL:HG13	1.85	0.54
1:A:261:SER:H	1:B:477:LYS:NZ	2.04	0.54
1:A:276:LEU:HD22	1:A:281:ARG:HE	1.71	0.54
1:B:430:ILE:HG13	1:B:430:ILE:O	2.08	0.53
1:B:257:VAL:HG12	1:B:290:VAL:HG22	1.90	0.53
1:A:294:LYS:HD2	1:A:295:LYS:NZ	2.23	0.53
1:B:279:GLY:O	1:B:286:ARG:NH2	2.41	0.53
1:A:67:GLN:O	1:A:71:GLU:HG3	2.09	0.53
1:B:393:PHE:CE2	1:B:397:LEU:HD21	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ASP:CG	1:B:319:PRO:HD3	2.34	0.52
1:A:393:PHE:H	2:A:501:EDO:H22	1.75	0.52
1:B:214:ARG:HD3	1:B:236:GLN:NE2	2.23	0.52
1:A:390:TYR:CD1	1:A:390:TYR:C	2.88	0.52
1:B:214:ARG:CG	1:B:236:GLN:NE2	2.73	0.52
1:B:258:GLN:HE22	4:B:501:MPD:CM	2.22	0.52
1:B:397:LEU:HD11	1:B:422:LEU:HA	1.91	0.52
1:A:134:VAL:HG12	1:A:136:ARG:CD	2.39	0.52
1:A:294:LYS:HG3	1:A:295:LYS:H	1.73	0.52
1:A:141:GLY:HA3	1:A:219:ASP:OD2	2.10	0.52
1:A:480:LEU:HD11	1:A:490:PHE:CE2	2.40	0.52
1:B:257:VAL:HG13	1:B:257:VAL:O	2.10	0.52
1:A:312:VAL:CG2	1:A:323:MET:HE2	2.40	0.52
1:A:456:ARG:HH11	4:B:502:MPD:H53	1.74	0.51
1:A:102:GLU:HG3	1:A:154:HIS:HB2	1.92	0.51
1:A:201:LEU:HD21	1:A:203:GLN:NE2	2.26	0.51
1:B:178:THR:O	1:B:181:VAL:HG12	2.10	0.51
1:B:353:MET:HE1	1:B:384:LEU:HB2	1.93	0.51
1:B:6:GLY:HA2	1:B:34:TRP:CZ2	2.46	0.51
1:B:257:VAL:HG11	1:B:299:PHE:CE2	2.46	0.50
1:B:294:LYS:HG3	1:B:295:LYS:CD	2.33	0.50
1:A:41:LEU:HD13	1:A:41:LEU:C	2.36	0.50
1:A:479:GLU:HA	1:B:265:GLY:HA3	1.93	0.50
1:A:353:MET:HE2	1:A:383:PRO:HG2	1.94	0.50
1:A:419:TYR:CD1	1:A:433:TRP:HB2	2.46	0.50
1:B:98:GLU:O	1:B:101:THR:HB	2.11	0.50
1:A:26:GLN:HG2	1:A:90:LEU:O	2.13	0.49
1:A:245:LEU:HD11	1:A:247:LEU:HD21	1.92	0.49
1:A:435:ARG:HD3	1:B:475:ALA:HB2	1.93	0.49
1:B:214:ARG:CG	1:B:236:GLN:HE22	2.25	0.49
1:A:24:SER:HB3	1:A:34:TRP:HB3	1.94	0.49
1:B:27:PRO:HB3	1:B:327:ILE:O	2.12	0.49
1:B:280:GLN:HE22	1:B:326:VAL:HA	1.77	0.49
1:B:78:GLU:HB2	1:B:107:MET:CE	2.43	0.48
1:B:96:LEU:HD23	1:B:316:ASP:HA	1.95	0.48
1:B:141:GLY:HA3	1:B:219:ASP:OD2	2.13	0.48
1:A:223:PHE:CZ	1:A:229:VAL:HG13	2.47	0.48
1:A:390:TYR:C	1:A:390:TYR:HD1	2.21	0.48
1:B:173:LYS:HE2	1:B:204:GLY:O	2.13	0.48
1:A:423:VAL:HG12	1:B:138:ARG:NH2	2.28	0.48
1:A:33:VAL:HG12	1:A:33:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ARG:NH2	1:B:455:HIS:O	2.47	0.48
1:B:125:GLU:HG3	1:B:134:VAL:HG22	1.95	0.48
1:A:214:ARG:CG	1:A:236:GLN:NE2	2.76	0.48
1:A:221:LEU:HD23	1:A:222:PHE:N	2.29	0.48
1:B:420:ASN:O	1:B:424:GLU:HG3	2.13	0.48
1:A:488:LEU:N	1:A:488:LEU:HD22	2.29	0.48
1:B:215:HIS:HE1	1:B:217:LEU:HD12	1.79	0.48
1:A:477:LYS:HE2	1:B:262:ASP:CB	2.44	0.47
1:B:290:VAL:HG13	1:B:291:PRO:HD2	1.96	0.47
1:B:140:HIS:N	1:B:168:ASN:OD1	2.45	0.47
1:B:214:ARG:HD3	1:B:236:GLN:HE21	1.80	0.47
1:A:39:ALA:HB3	1:A:202:VAL:CG1	2.40	0.47
1:B:422:LEU:CD1	1:B:426:VAL:HB	2.43	0.47
1:A:276:LEU:HD23	1:A:277:SER:N	2.29	0.47
1:A:280:GLN:HE22	1:A:326:VAL:HA	1.76	0.47
1:A:309:ARG:HD3	1:B:489:ASN:HB3	1.96	0.47
1:B:285:ALA:CB	1:B:437:LEU:HD12	2.39	0.47
1:A:256:ILE:O	1:A:411:ILE:HA	2.15	0.47
1:A:201:LEU:HD21	1:A:203:GLN:HE21	1.78	0.47
1:A:210:LYS:HD3	1:A:214:ARG:NH2	2.30	0.47
1:B:421:ARG:HH22	4:B:501:MPD:C1	2.28	0.47
1:A:173:LYS:HD3	1:A:173:LYS:C	2.39	0.46
1:A:78:GLU:HB2	1:A:107:MET:HE3	1.97	0.46
1:B:94:LYS:NZ	1:B:102:GLU:OE1	2.47	0.46
1:A:470:MET:HG3	1:B:428:ALA:O	2.14	0.46
1:B:26:GLN:HG2	1:B:90:LEU:O	2.15	0.46
1:B:41:LEU:HD23	1:B:41:LEU:C	2.40	0.46
4:B:501:MPD:H53	4:B:501:MPD:O2	2.16	0.46
1:A:265:GLY:HA3	1:B:479:GLU:HA	1.98	0.46
1:A:286:ARG:HD2	1:A:380:PHE:CE1	2.51	0.46
1:B:177:LEU:HD13	1:B:327:ILE:HG12	1.96	0.46
1:A:138:ARG:HH21	1:B:423:VAL:HG12	1.81	0.46
1:B:392:GLY:O	1:B:395:GLU:HB3	2.16	0.46
1:A:420:ASN:O	1:A:424:GLU:HG3	2.16	0.46
1:B:78:GLU:HB2	1:B:107:MET:HE3	1.98	0.46
1:A:332:ALA:O	1:A:336:LEU:HD22	2.16	0.45
1:A:332:ALA:HB1	1:A:363:LEU:HD21	1.97	0.45
1:A:486:PRO:O	1:B:322:PHE:HB2	2.16	0.45
1:B:24:SER:HB3	1:B:34:TRP:HB3	1.97	0.45
1:B:286:ARG:NE	1:B:380:PHE:O	2.50	0.45
1:A:414:ASP:OD1	1:B:477:LYS:CD	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ARG:NH1	1:B:217:LEU:HD22	2.31	0.45
1:B:421:ARG:HH22	4:B:501:MPD:H11	1.81	0.45
1:A:221:LEU:HD23	1:A:221:LEU:C	2.41	0.45
1:B:21:PRO:HA	1:B:36:GLY:O	2.15	0.45
1:B:295:LYS:O	1:B:298:GLU:OE2	2.35	0.45
1:B:260:VAL:HG11	1:B:266:ALA:HB2	1.98	0.45
1:A:98:GLU:O	1:A:101:THR:HB	2.17	0.45
1:A:285:ALA:HB2	1:A:437:LEU:HD12	1.99	0.45
1:A:29:THR:HG22	1:A:31:GLU:N	2.29	0.44
1:A:294:LYS:HD2	1:A:295:LYS:HZ2	1.82	0.44
1:A:332:ALA:CB	1:A:363:LEU:HD21	2.47	0.44
1:A:335:LEU:HD21	1:A:382:GLY:CA	2.43	0.44
1:A:430:ILE:O	1:A:430:ILE:HG13	2.18	0.44
1:B:202:VAL:HG23	1:B:202:VAL:O	2.17	0.44
1:A:138:ARG:HB2	1:A:468:TRP:CE2	2.53	0.44
1:A:143:VAL:HA	1:A:220:GLY:O	2.18	0.44
1:B:95:PRO:HB2	1:B:97:TRP:CD1	2.53	0.44
1:A:350:LEU:CD1	1:A:369:ASP:HB2	2.48	0.43
1:B:347:ALA:HB1	1:B:368:VAL:CG1	2.48	0.43
4:B:502:MPD:O4	4:B:502:MPD:H11	2.18	0.43
1:B:26:GLN:OE1	1:B:28:VAL:CG1	2.66	0.43
1:B:215:HIS:CE1	1:B:217:LEU:HB2	2.54	0.43
1:A:345:LYS:HE3	1:A:345:LYS:HB2	1.80	0.43
1:A:221:LEU:HB3	1:A:245:LEU:HD23	2.01	0.43
1:B:97:TRP:HZ2	1:B:322:PHE:O	2.02	0.43
1:A:489:ASN:C	1:A:490:PHE:HD1	2.26	0.43
1:B:153:GLY:O	1:B:157:ASN:HB2	2.19	0.43
1:A:313:ALA:HB3	1:A:321:PRO:HG3	2.01	0.42
1:B:210:LYS:HD3	1:B:214:ARG:NH2	2.20	0.42
1:B:96:LEU:HB3	1:B:100:ARG:CZ	2.49	0.42
1:A:228:THR:O	1:A:232:LEU:CD2	2.66	0.42
1:A:125:GLU:HG2	1:A:134:VAL:HG22	2.00	0.42
1:A:371:THR:OG1	1:A:389:ARG:HG2	2.19	0.42
1:B:254:PRO:HA	1:B:287:ARG:O	2.18	0.42
1:B:128:VAL:HG13	1:B:129:ALA:N	2.34	0.42
1:A:194:LEU:HD23	1:A:199:ILE:HG22	2.01	0.42
1:A:417:LYS:HD2	1:A:420:ASN:HB2	2.01	0.42
1:B:9:TYR:HB2	1:B:14:TRP:CZ3	2.55	0.42
1:B:312:VAL:HG21	1:B:323:MET:HE2	2.00	0.42
1:B:221:LEU:HD23	1:B:221:LEU:C	2.45	0.42
1:A:258:GLN:O	1:A:259:ASN:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ALA:O	1:A:335:LEU:HD13	2.19	0.41
1:A:353:MET:HE1	1:A:384:LEU:HB2	2.02	0.41
1:A:78:GLU:HB2	1:A:107:MET:HE1	2.02	0.41
1:B:267:VAL:HG13	1:B:303:LEU:HA	2.01	0.41
1:A:437:LEU:HD23	1:A:437:LEU:HA	1.83	0.41
1:A:477:LYS:HZ3	1:B:262:ASP:HB2	1.85	0.41
1:B:70:ILE:O	1:B:73:PHE:HB3	2.20	0.41
1:A:174:PRO:HG2	1:A:203:GLN:OE1	2.20	0.41
1:A:298:GLU:HG3	1:A:299:PHE:H	1.86	0.41
1:A:351:LEU:HD23	1:A:352:GLU:N	2.36	0.41
4:B:501:MPD:O4	4:B:501:MPD:C1	2.67	0.41
1:A:194:LEU:HD23	1:A:199:ILE:CG2	2.51	0.41
1:B:355:GLN:HA	1:B:363:LEU:HD12	2.02	0.41
1:B:353:MET:CE	1:B:384:LEU:HB2	2.51	0.41
1:A:8:VAL:CG1	1:A:10:ILE:HG13	2.50	0.41
1:A:286:ARG:HA	1:A:286:ARG:HD3	1.67	0.41
1:A:369:ASP:OD1	1:A:371:THR:OG1	2.34	0.41
1:B:96:LEU:O	1:B:100:ARG:HG3	2.21	0.41
1:A:112:ILE:HD12	1:A:112:ILE:HA	1.90	0.40
1:B:33:VAL:O	1:B:33:VAL:HG12	2.22	0.40
1:B:330:GLU:O	1:B:333:ASN:HB3	2.21	0.40
1:A:125:GLU:HA	1:A:133:ALA:O	2.21	0.40
1:B:9:TYR:HB3	1:B:201:LEU:HB3	2.03	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	486/497 (98%)	465 (96%)	21 (4%)	0	100	100
1	B	485/497 (98%)	463 (96%)	22 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	971/994 (98%)	928 (96%)	43 (4%)	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	378/386 (98%)	364 (96%)	14 (4%)	30	43
1	B	377/386 (98%)	367 (97%)	10 (3%)	39	55
All	All	755/772 (98%)	731 (97%)	24 (3%)	34	49

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	29	THR
1	A	165	LEU
1	A	245	LEU
1	A	309	ARG
1	A	318	ASP
1	A	336	LEU
1	A	348	THR
1	A	356	LEU
1	A	363	LEU
1	A	380	PHE
1	A	390	TYR
1	A	397	LEU
1	A	430	ILE
1	B	4	LEU
1	B	28	VAL
1	B	96	LEU
1	B	128	VAL
1	B	136	ARG
1	B	165	LEU

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Mol	Chain	Res	Type
1	B	229	VAL
1	B	318	ASP
1	B	363	LEU
1	B	488	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	A	252	ASN
1	A	258	GLN
1	A	259	ASN
1	A	280	GLN
1	B	86	HIS
1	B	140	HIS
1	B	154	HIS
1	B	236	GLN
1	B	258	GLN
1	B	272	GLN
1	B	378	GLN

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](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	A	504	-	3,3,3	0.40	0	2,2,2	0.55	0
2	EDO	A	506	-	3,3,3	0.67	0	2,2,2	0.02	0
2	EDO	A	503	-	3,3,3	0.45	0	2,2,2	0.26	0
2	EDO	A	505	-	3,3,3	0.66	0	2,2,2	0.14	0
4	MPD	B	502	-	7,7,7	0.68	0	9,10,10	0.70	0
2	EDO	A	502	-	3,3,3	0.55	0	2,2,2	0.22	0
2	EDO	A	508	-	3,3,3	0.47	0	2,2,2	0.48	0
4	MPD	B	501	-	7,7,7	0.54	0	9,10,10	0.69	0
6	PO4	B	504	-	4,4,4	0.77	0	6,6,6	0.79	0
3	8YP	A	507	-	7,7,10	0.59	0	6,6,9	0.66	0
2	EDO	A	509	-	3,3,3	0.67	0	2,2,2	0.19	0
2	EDO	A	501	-	3,3,3	0.66	0	2,2,2	0.07	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	A	504	-	-	1/1/1/1	-
2	EDO	A	506	-	-	1/1/1/1	-
2	EDO	A	503	-	-	1/1/1/1	-
2	EDO	A	505	-	-	1/1/1/1	-
4	MPD	B	502	-	-	1/5/5/5	-
2	EDO	A	502	-	-	1/1/1/1	-
2	EDO	A	508	-	-	0/1/1/1	-
4	MPD	B	501	-	-	1/5/5/5	-
3	8YP	A	507	-	-	4/5/5/8	-
2	EDO	A	509	-	-	1/1/1/1	-
2	EDO	A	501	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	MPD	C2-C3-C4-C5
2	A	502	EDO	O1-C1-C2-O2
2	A	506	EDO	O1-C1-C2-O2
3	A	507	8YP	C1-C2-C3-C4
3	A	507	8YP	C5-C6-C7-C8
2	A	503	EDO	O1-C1-C2-O2
3	A	507	8YP	C2-C3-C4-C5
2	A	505	EDO	O1-C1-C2-O2
2	A	504	EDO	O1-C1-C2-O2
2	A	501	EDO	O1-C1-C2-O2
3	A	507	8YP	C4-C5-C6-C7
2	A	509	EDO	O1-C1-C2-O2
4	B	502	MPD	O2-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	505	EDO	1	0
4	B	502	MPD	3	0
4	B	501	MPD	12	0
2	A	501	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	488/497 (98%)	0.11	6 (1%) 76 78	47, 64, 93, 127	0
1	B	487/497 (97%)	0.33	7 (1%) 73 75	47, 75, 111, 152	0
All	All	975/994 (98%)	0.22	13 (1%) 75 76	47, 68, 106, 152	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	LEU	5.8
1	A	490	PHE	5.1
1	A	380	PHE	3.8
1	B	295	LYS	3.6
1	B	490	PHE	3.3
1	B	151	PHE	2.4
1	A	136	ARG	2.4
1	B	294	LYS	2.3
1	B	476	GLY	2.2
1	A	371	THR	2.2
1	A	488	LEU	2.1
1	A	294	LYS	2.1
1	B	319	PRO	2.1

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
4	MPD	B	501	8/8	0.63	0.21	75,77,80,84	0
2	EDO	A	501	4/4	0.64	0.18	76,91,96,98	0
3	8YP	A	507	8/11	0.69	0.24	61,83,91,92	0
6	PO4	B	504	5/5	0.69	0.13	104,105,107,108	0
2	EDO	A	504	4/4	0.74	0.22	85,103,106,108	0
2	EDO	A	503	4/4	0.74	0.15	89,107,113,113	0
2	EDO	A	505	4/4	0.78	0.20	67,81,83,88	0
2	EDO	A	502	4/4	0.78	0.18	80,96,98,99	0
4	MPD	B	502	8/8	0.79	0.26	83,88,90,91	0
2	EDO	A	506	4/4	0.79	0.24	68,87,97,105	0
2	EDO	A	509	4/4	0.81	0.22	94,113,119,119	0
5	CL	B	503	1/1	0.88	0.19	104,104,104,104	0
2	EDO	A	508	4/4	0.88	0.17	91,110,110,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.