



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:33 PM UTC

PDB ID : 6N01 / pdb_00006n01
Title : Structure of apo AztD from *Citrobacter koseri*
Authors : Yukl, E.T.; Neupane, D.P.
Deposited on : 2018-11-06
Resolution : 1.98 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

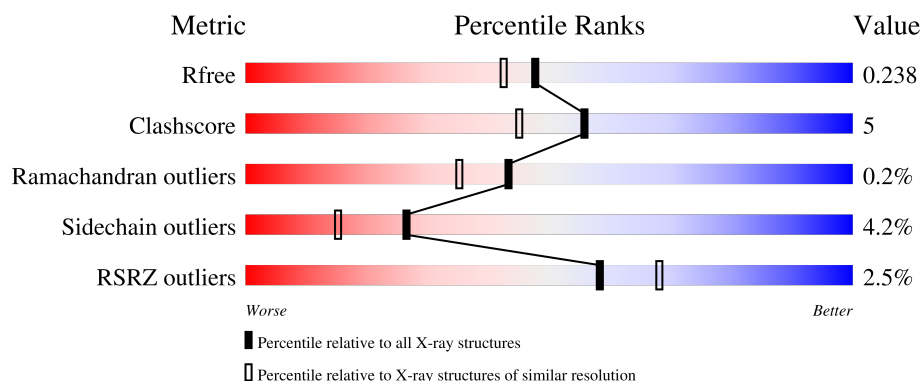
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	421	% 76% 10% • 13%
1	B	421	3% 74% 10% • 14%
1	C	421	4% 78% 8% • 13%
1	D	421	% 77% 10% 13%

2 Entry composition [i](#)

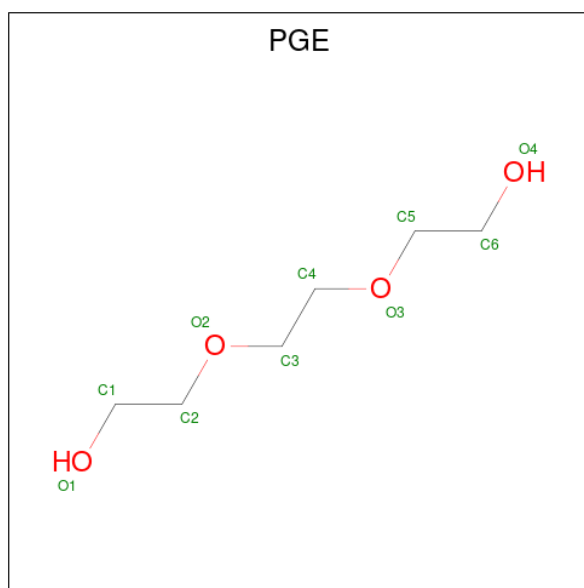
There are 5 unique types of molecules in this entry. The entry contains 22318 atoms, of which 10707 are hydrogens and 0 are deuteriums.

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 AztD Protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	361	Total	C	H	N	O	S	0	3	0
			5420	1743	2679	473	521	4			
1	A	367	Total	C	H	N	O	S	0	1	0
			5432	1763	2653	481	531	4			
1	C	367	Total	C	H	N	O	S	0	0	0
			5436	1763	2661	480	528	4			
1	D	367	Total	C	H	N	O	S	0	0	0
			5436	1763	2661	480	528	4			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



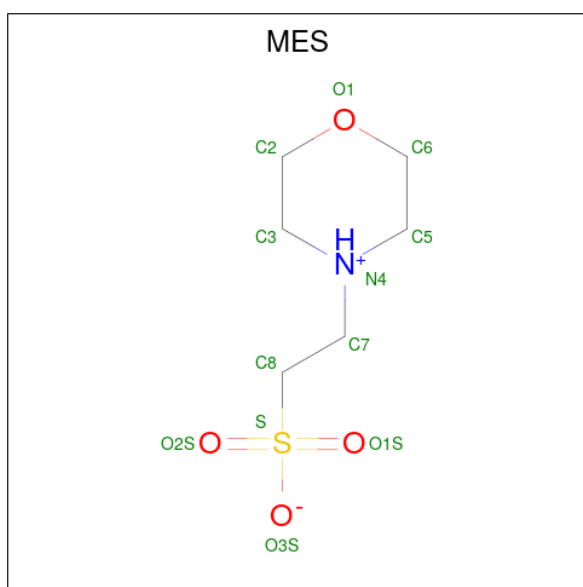
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			24	6	14	4		
2	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	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	D	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

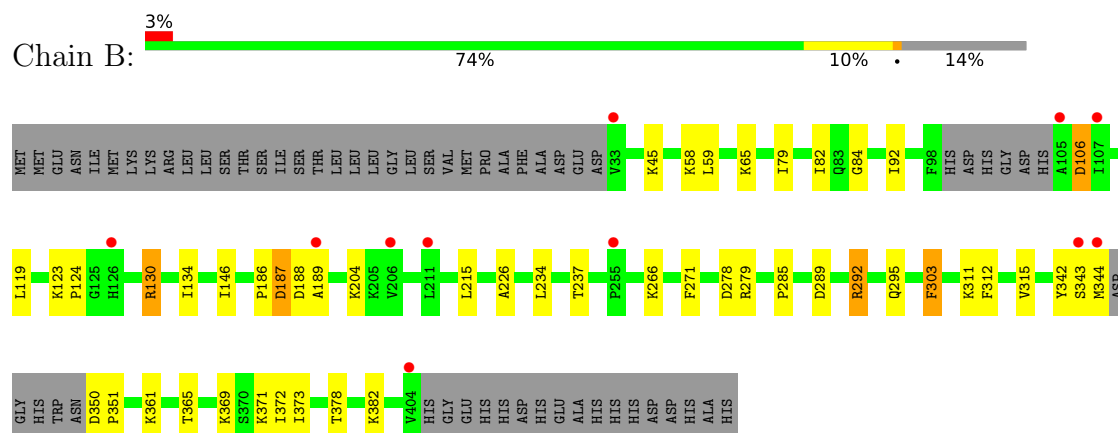
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	110	Total	O	0	0
			110	110		
5	A	151	Total	O	0	0
			151	151		
5	C	97	Total	O	0	0
			97	97		
5	D	143	Total	O	0	0
			143	143		

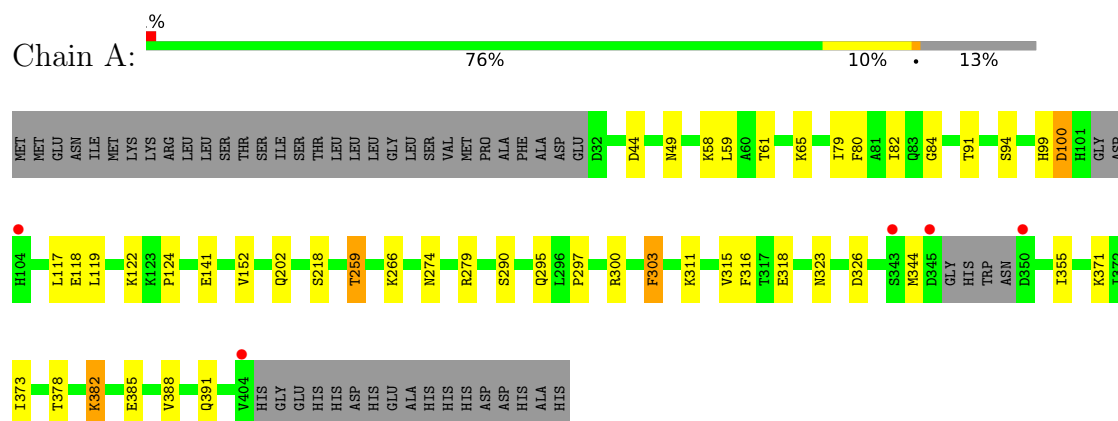
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

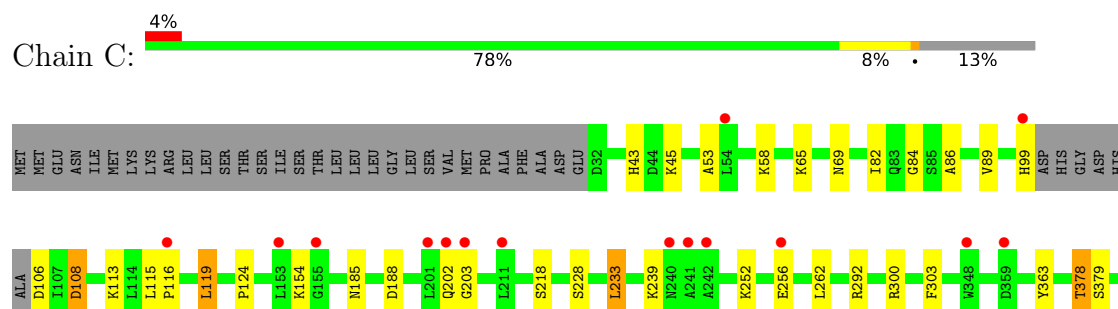
• Molecule 1: AztD Protein

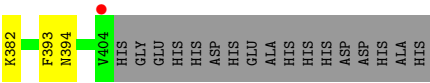


• Molecule 1: AztD Protein

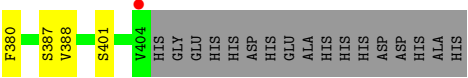
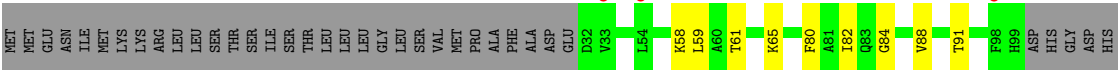
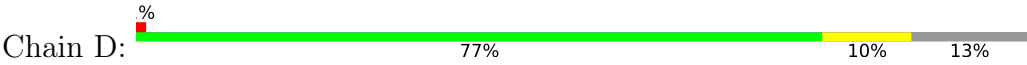


• Molecule 1: AztD Protein





● Molecule 1: AztD Protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.87Å 127.85Å 113.16Å 90.00° 94.51° 90.00°	Depositor
Resolution (Å)	48.43 – 1.98 48.43 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.43-1.98) 98.5 (48.43-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.98Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.195 , 0.238 0.196 , 0.238	Depositor DCC
R_{free} test set	2004 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22318	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0246e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, 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	0.61	0/2835	0.74	0/3852
1	B	0.55	0/2795	0.70	0/3797
1	C	0.51	0/2833	0.68	0/3851
1	D	0.62	0/2833	0.76	1/3851 (0.0%)
All	All	0.57	0/11296	0.72	1/15351 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	355	ILE	CB-CA-C	-5.24	102.52	110.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2779	2653	2793	28	0
1	B	2741	2679	2772	30	0
1	C	2775	2661	2791	21	0
1	D	2775	2661	2791	23	0
2	A	10	14	14	2	0
2	B	10	14	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4	6	6	1	0
3	D	4	6	6	1	0
4	D	12	13	13	2	0
5	A	151	0	0	7	0
5	B	110	0	0	9	0
5	C	97	0	0	6	0
5	D	143	0	0	7	0
All	All	11611	10707	11200	105	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 (105) 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:65:LYS:NZ	1:A:118:GLU:OE2	2.05	0.88
1:A:99:HIS:O	1:A:100:ASP:HB2	1.72	0.86
1:C:256:GLU:HG3	3:C:501:EDO:H11	1.57	0.86
1:B:303:PHE:HB3	1:B:315[A]:VAL:HG12	1.57	0.85
4:D:501:MES:O1S	5:D:601:HOH:O	1.97	0.83
1:C:218:SER:O	5:C:601:HOH:O	2.09	0.70
1:D:310:ALA:O	5:D:602:HOH:O	2.09	0.69
1:A:326:ASP:OD1	5:A:601:HOH:O	2.14	0.66
1:C:262:LEU:O	5:C:601:HOH:O	2.12	0.66
1:D:65:LYS:NZ	1:D:118:GLU:OE2	2.24	0.65
1:A:259:THR:HB	1:A:274:ASN:O	1.95	0.65
1:B:186:PRO:O	1:B:187:ASP:HB2	1.99	0.63
1:A:122:LYS:HE3	1:A:141:GLU:OE2	2.00	0.62
1:D:176:ASP:OD2	5:D:603:HOH:O	2.16	0.61
1:C:300:ARG:NH1	5:C:602:HOH:O	2.33	0.60
1:C:53:ALA:O	1:C:363:TYR:OH	2.19	0.60
1:A:91:THR:HG21	1:A:117:LEU:HD23	1.85	0.58
1:D:373:ILE:HD12	1:D:373:ILE:N	2.19	0.57
1:D:256:GLU:HB3	3:D:502:EDO:H12	1.87	0.57
1:A:279:ARG:HD3	1:A:295:GLN:OE1	2.05	0.56
1:C:89:VAL:HB	1:C:119:LEU:HB2	1.87	0.56
1:B:373:ILE:HG23	1:B:382:LYS:HD2	1.87	0.56
1:A:297:PRO:HG2	5:A:604:HOH:O	2.07	0.55
1:A:373:ILE:HG23	1:A:382:LYS:HD2	1.87	0.55
1:D:365:THR:HG22	1:D:372:ILE:HD12	1.89	0.55
1:B:342:TYR:O	1:B:344:MET:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:LYS:NZ	5:B:602:HOH:O	2.27	0.54
1:A:371:LYS:HE3	1:A:373:ILE:HD11	1.89	0.54
2:A:501:PGE:C2	5:A:609:HOH:O	2.56	0.54
1:D:300:ARG:NH1	5:D:618:HOH:O	2.40	0.53
1:A:82:ILE:HG23	1:A:124:PRO:HB2	1.89	0.53
1:D:344:MET:O	4:D:501:MES:H32	2.09	0.53
1:B:130:ARG:HD2	5:B:703:HOH:O	2.09	0.53
1:B:271:PHE:CE2	1:B:285:PRO:HG3	2.45	0.52
1:B:279:ARG:NH1	5:B:601:HOH:O	2.24	0.52
2:A:501:PGE:H22	5:A:609:HOH:O	2.10	0.52
1:B:311:LYS:HE3	1:B:312:PHE:CE2	2.46	0.51
1:D:237:THR:HG22	5:D:646:HOH:O	2.09	0.51
1:C:82:ILE:HG23	1:C:124:PRO:HB2	1.91	0.51
1:D:387:SER:OG	5:D:604:HOH:O	2.19	0.51
1:A:117:LEU:HD22	1:A:152:VAL:HG22	1.93	0.50
1:A:79:ILE:CD1	1:A:94:SER:HB3	2.41	0.50
1:D:205:LYS:HE3	1:D:209:ASP:OD1	2.12	0.49
1:A:303:PHE:HB3	1:A:315:VAL:HG12	1.95	0.49
1:B:82:ILE:HG23	1:B:124:PRO:HB2	1.94	0.49
1:D:197:ARG:HD3	1:D:205:LYS:HG2	1.95	0.49
1:D:117:LEU:HD13	1:D:157:LYS:HB2	1.93	0.48
1:B:130:ARG:HG2	5:B:703:HOH:O	2.13	0.48
1:A:316:PHE:HB2	1:A:355:ILE:HD11	1.95	0.48
1:B:350:ASP:N	1:B:351:PRO:CD	2.77	0.48
1:B:186:PRO:O	1:B:187:ASP:CB	2.62	0.48
1:B:278:ASP:OD2	1:B:295:GLN:NE2	2.43	0.48
1:C:69:ASN:ND2	1:C:394:ASN:OD1	2.45	0.47
1:B:130:ARG:CG	5:B:703:HOH:O	2.62	0.47
1:A:218:SER:O	5:A:603:HOH:O	2.21	0.47
1:A:382:LYS:NZ	1:A:385:GLU:HG3	2.30	0.47
1:D:373:ILE:N	1:D:373:ILE:CD1	2.77	0.46
1:B:84:GLY:HA2	1:B:124:PRO:HD2	1.97	0.46
1:C:382:LYS:NZ	5:C:611:HOH:O	2.48	0.46
1:B:371:LYS:HE3	1:B:373:ILE:HD11	1.97	0.46
1:D:82:ILE:HG23	1:D:124:PRO:HB2	1.97	0.46
1:B:188:ASP:O	1:B:189:ALA:HB3	2.16	0.46
1:A:344:MET:HE1	5:A:737:HOH:O	2.16	0.46
1:C:99:HIS:NE2	1:C:108:ASP:OD2	2.49	0.46
1:A:44:ASP:OD2	1:A:391:GLN:OE1	2.34	0.45
1:B:79:ILE:HB	1:B:92:ILE:HB	1.98	0.45
1:D:117:LEU:CD2	1:D:152:VAL:HG13	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLU:HG3	1:A:344:MET:HG2	1.99	0.45
1:D:122:LYS:HD3	1:D:141:GLU:OE2	2.17	0.45
1:D:360:ASN:ND2	5:D:626:HOH:O	2.50	0.44
1:A:300:ARG:NH1	5:A:616:HOH:O	2.45	0.44
1:D:80:PHE:CD2	1:D:91:THR:HG22	2.52	0.44
1:C:202:GLN:N	1:C:203:GLY:HA2	2.32	0.44
1:C:292:ARG:NH2	5:C:605:HOH:O	2.40	0.44
1:B:365:THR:HG22	1:B:372:ILE:CD1	2.48	0.43
1:B:237:THR:HG22	5:B:637:HOH:O	2.17	0.43
1:C:228:SER:HA	1:C:233:LEU:HD12	2.01	0.43
1:A:84:GLY:HA2	1:A:124:PRO:HD2	2.01	0.43
1:C:378:THR:HG22	1:C:379:SER:N	2.33	0.43
1:D:365:THR:HG22	1:D:372:ILE:CD1	2.47	0.43
1:C:185:ASN:HB3	1:C:188:ASP:O	2.18	0.42
1:A:49:ASN:OD1	1:A:61:THR:HG22	2.18	0.42
1:A:315:VAL:CG2	1:A:323:ASN:HB2	2.48	0.42
1:C:115:LEU:HB3	1:C:116:PRO:HD2	2.00	0.42
1:B:106:ASP:OD1	1:B:106:ASP:N	2.52	0.42
1:B:130:ARG:NH1	5:B:612:HOH:O	2.51	0.42
1:C:202:GLN:H	1:C:203:GLY:HA2	1.85	0.42
1:C:84:GLY:HA2	1:C:124:PRO:HD2	2.01	0.42
1:B:215:LEU:C	1:B:215:LEU:HD23	2.44	0.42
1:A:311:LYS:HB2	1:A:311:LYS:HE3	1.90	0.41
1:D:185:ASN:HB3	1:D:188:ASP:O	2.20	0.41
1:D:239:LYS:HB2	1:D:240:ASN:H	1.66	0.41
1:B:289:ASP:OD1	1:B:292:ARG:NH2	2.53	0.41
1:B:365:THR:HG22	1:B:372:ILE:HD12	2.01	0.41
1:A:80:PHE:CD2	1:A:91:THR:HG22	2.55	0.41
1:C:65:LYS:HB3	1:C:86:ALA:HB1	2.03	0.41
1:B:134:ILE:O	1:B:146:ILE:HA	2.21	0.41
1:B:226:ALA:HA	1:B:234:LEU:O	2.21	0.41
1:C:292:ARG:NE	5:C:605:HOH:O	2.45	0.41
1:B:130:ARG:CD	5:B:703:HOH:O	2.68	0.40
1:C:43:HIS:HB2	1:C:393:PHE:HB2	2.03	0.40
1:A:117:LEU:CD2	1:A:152:VAL:HG22	2.51	0.40
1:B:237:THR:HG23	5:B:696:HOH:O	2.21	0.40
1:A:82:ILE:N	1:A:82:ILE:HD12	2.37	0.40
1:D:84:GLY:HA2	1:D:124:PRO:HD2	2.04	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	362/421 (86%)	348 (96%)	13 (4%)	1 (0%)	36	27
1	B	358/421 (85%)	344 (96%)	12 (3%)	2 (1%)	21	12
1	C	363/421 (86%)	351 (97%)	12 (3%)	0	100	100
1	D	363/421 (86%)	354 (98%)	9 (2%)	0	100	100
All	All	1446/1684 (86%)	1397 (97%)	46 (3%)	3 (0%)	43	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	343	SER
1	A	100	ASP
1	B	187	ASP

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	303/348 (87%)	292 (96%)	11 (4%)	31	20
1	B	299/348 (86%)	285 (95%)	14 (5%)	23	12
1	C	302/348 (87%)	290 (96%)	12 (4%)	28	17
1	D	302/348 (87%)	288 (95%)	14 (5%)	24	12
All	All	1206/1392 (87%)	1155 (96%)	51 (4%)	26	15

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45	LYS
1	B	58	LYS
1	B	59	LEU
1	B	65	LYS
1	B	106	ASP
1	B	119	LEU
1	B	123	LYS
1	B	130	ARG
1	B	204	LYS
1	B	266	LYS
1	B	292	ARG
1	B	303	PHE
1	B	361	LYS
1	B	378	THR
1	A	58	LYS
1	A	59	LEU
1	A	119	LEU
1	A	202	GLN
1	A	259	THR
1	A	266	LYS
1	A	290	SER
1	A	303	PHE
1	A	378	THR
1	A	382	LYS
1	A	388	VAL
1	C	45	LYS
1	C	58	LYS
1	C	106	ASP
1	C	108	ASP
1	C	113	LYS
1	C	119	LEU
1	C	154	LYS
1	C	233	LEU
1	C	239	LYS
1	C	252	LYS
1	C	303	PHE
1	C	378	THR
1	D	58	LYS
1	D	59	LEU
1	D	61	THR
1	D	88	VAL
1	D	126	HIS
1	D	130	ARG

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Mol	Chain	Res	Type
1	D	147	LEU
1	D	205	LYS
1	D	303	PHE
1	D	373	ILE
1	D	378	THR
1	D	380	PHE
1	D	388	VAL
1	D	401	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	391	GLN
1	A	104	HIS
1	A	177	ASN
1	C	324	GLN
1	C	334	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](#)

5 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	$\# Z > 2$
2	PGE	B	501	-	9,9,9	0.32	0	8,8,8	0.60	0
2	PGE	A	501	-	9,9,9	0.38	0	8,8,8	0.60	0
3	EDO	C	501	-	3,3,3	0.29	0	2,2,2	0.51	0
4	MES	D	501	-	12,12,12	2.16	1 (8%)	15,16,16	1.55	3 (20%)
3	EDO	D	502	-	3,3,3	0.56	0	2,2,2	0.74	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	PGE	B	501	-	-	4/7/7/7	-
2	PGE	A	501	-	-	3/7/7/7	-
3	EDO	C	501	-	-	1/1/1/1	-
4	MES	D	501	-	-	3/6/14/14	0/1/1/1
3	EDO	D	502	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	MES	C8-S	-7.10	1.67	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	MES	O1S-S-C8	3.93	112.66	106.73
4	D	501	MES	C5-N4-C3	2.68	114.61	108.84
4	D	501	MES	O2S-S-C8	2.50	110.51	106.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	501	MES	C7-C8-S-O3S
2	B	501	PGE	O1-C1-C2-O2
4	D	501	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
4	D	501	MES	C7-C8-S-O2S
2	B	501	PGE	C4-C3-O2-C2
2	A	501	PGE	C1-C2-O2-C3
2	A	501	PGE	O3-C5-C6-O4
3	C	501	EDO	O1-C1-C2-O2
2	A	501	PGE	C4-C3-O2-C2
2	B	501	PGE	O3-C5-C6-O4
2	B	501	PGE	C6-C5-O3-C4

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PGE	2	0
3	C	501	EDO	1	0
4	D	501	MES	2	0
3	D	502	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	367/421 (87%)	-0.02	5 (1%) 73 81	13, 36, 61, 76	1 (0%)
1	B	361/421 (85%)	0.26	11 (3%) 52 62	16, 42, 68, 89	3 (0%)
1	C	367/421 (87%)	0.30	16 (4%) 39 49	25, 45, 75, 92	0
1	D	367/421 (87%)	0.02	5 (1%) 73 81	20, 37, 62, 83	0
All	All	1462/1684 (86%)	0.14	37 (2%) 58 68	13, 40, 67, 92	4 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	ALA	4.6
1	C	54	LEU	4.5
1	D	117	LEU	3.8
1	D	404	VAL	3.7
1	B	344	MET	3.5
1	A	343	SER	3.3
1	C	201	LEU	3.3
1	B	126[A]	HIS	3.3
1	C	240	ASN	3.2
1	B	404	VAL	3.2
1	B	33	VAL	2.9
1	C	116	PRO	2.8
1	C	348	TRP	2.7
1	D	54	LEU	2.6
1	C	404	VAL	2.6
1	C	155	GLY	2.5
1	A	345	ASP	2.5
1	D	33	VAL	2.5
1	B	189	ALA	2.3
1	D	98	PHE	2.3
1	C	241	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	242	ALA	2.3
1	A	104	HIS	2.3
1	B	343	SER	2.2
1	C	211	LEU	2.2
1	B	107	ILE	2.2
1	C	99	HIS	2.2
1	C	256	GLU	2.2
1	C	202	GLN	2.1
1	B	255	PRO	2.1
1	B	206	VAL	2.1
1	C	359	ASP	2.1
1	A	350	ASP	2.1
1	A	404	VAL	2.0
1	B	211	LEU	2.0
1	C	153	LEU	2.0
1	C	203	GLY	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	PGE	B	501	10/10	0.86	0.14	46,58,70,73	0
3	EDO	C	501	4/4	0.86	0.17	43,59,71,71	0
3	EDO	D	502	4/4	0.87	0.15	31,38,50,60	0
4	MES	D	501	12/12	0.92	0.09	35,49,62,71	0
2	PGE	A	501	10/10	0.94	0.10	35,47,76,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.