



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 11:04 PM BST

PDB ID : 5WZE
Title : The structure of Pseudomonas aeruginosa aminopeptidase PepP
Authors : Bao, R.; Peng, C.T.; Liu, L.; He, L.H.; Li, C.C.; Li, T.; Shen, Y.L.; Zhu, Y.B.;
Song, Y.J.
Deposited on : 2017-01-17
Resolution : 1.78 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

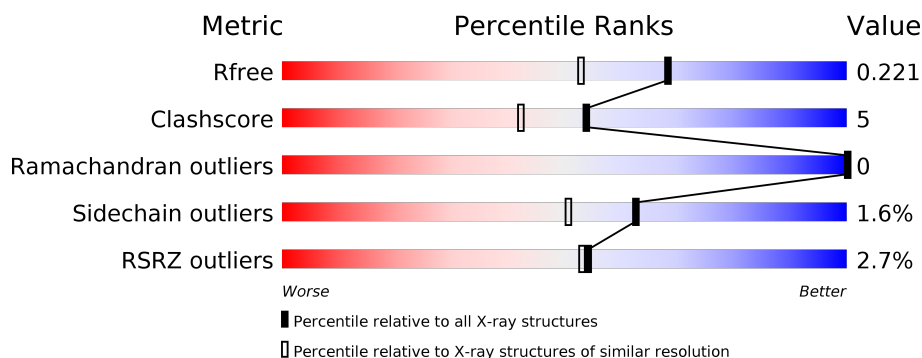
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 on 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	452	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>.</div> </div> </div>
1	B	452	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
1	C	452	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	D	452	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>..</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	EDO	B	505	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15378 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 Aminopeptidase P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	4	0
			3511	2217	627	645	22			
1	B	449	Total	C	N	O	S	0	4	0
			3550	2244	631	654	21			
1	C	442	Total	C	N	O	S	0	7	0
			3523	2229	630	643	21			
1	D	444	Total	C	N	O	S	0	3	0
			3509	2217	624	647	21			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	LEU	-	expression tag	UNP Q9HTW6
A	446	GLU	-	expression tag	UNP Q9HTW6
A	447	HIS	-	expression tag	UNP Q9HTW6
A	448	HIS	-	expression tag	UNP Q9HTW6
A	449	HIS	-	expression tag	UNP Q9HTW6
A	450	HIS	-	expression tag	UNP Q9HTW6
A	451	HIS	-	expression tag	UNP Q9HTW6
A	452	HIS	-	expression tag	UNP Q9HTW6
B	445	LEU	-	expression tag	UNP Q9HTW6
B	446	GLU	-	expression tag	UNP Q9HTW6
B	447	HIS	-	expression tag	UNP Q9HTW6
B	448	HIS	-	expression tag	UNP Q9HTW6
B	449	HIS	-	expression tag	UNP Q9HTW6
B	450	HIS	-	expression tag	UNP Q9HTW6
B	451	HIS	-	expression tag	UNP Q9HTW6
B	452	HIS	-	expression tag	UNP Q9HTW6
C	445	LEU	-	expression tag	UNP Q9HTW6
C	446	GLU	-	expression tag	UNP Q9HTW6
C	447	HIS	-	expression tag	UNP Q9HTW6
C	448	HIS	-	expression tag	UNP Q9HTW6
C	449	HIS	-	expression tag	UNP Q9HTW6

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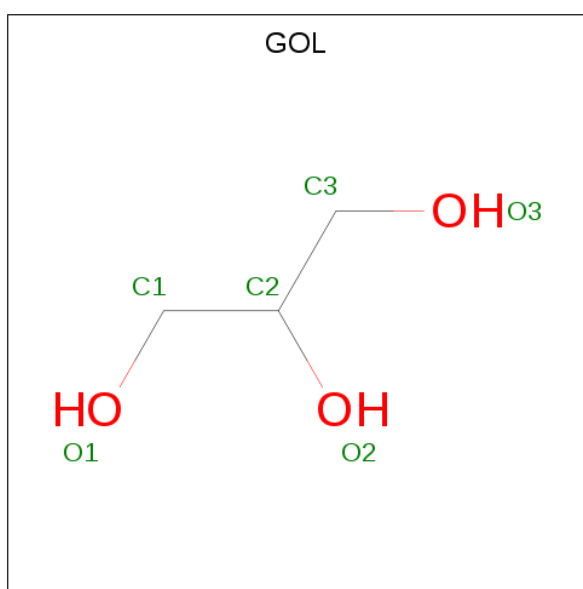
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Chain	Residue	Modelled	Actual	Comment	Reference
C	450	HIS	-	expression tag	UNP Q9HTW6
C	451	HIS	-	expression tag	UNP Q9HTW6
C	452	HIS	-	expression tag	UNP Q9HTW6
D	445	LEU	-	expression tag	UNP Q9HTW6
D	446	GLU	-	expression tag	UNP Q9HTW6
D	447	HIS	-	expression tag	UNP Q9HTW6
D	448	HIS	-	expression tag	UNP Q9HTW6
D	449	HIS	-	expression tag	UNP Q9HTW6
D	450	HIS	-	expression tag	UNP Q9HTW6
D	451	HIS	-	expression tag	UNP Q9HTW6
D	452	HIS	-	expression tag	UNP Q9HTW6

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

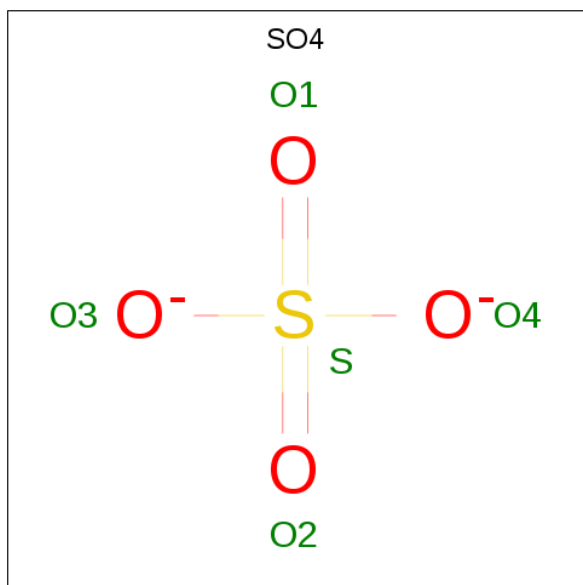
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Na 2 2	0	0
2	A	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



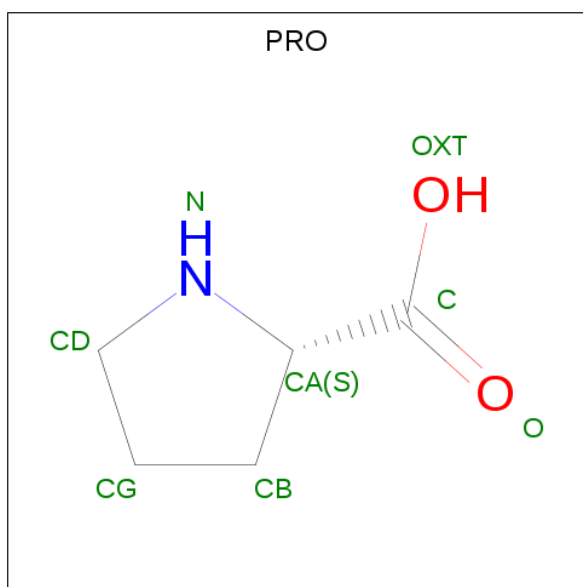
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



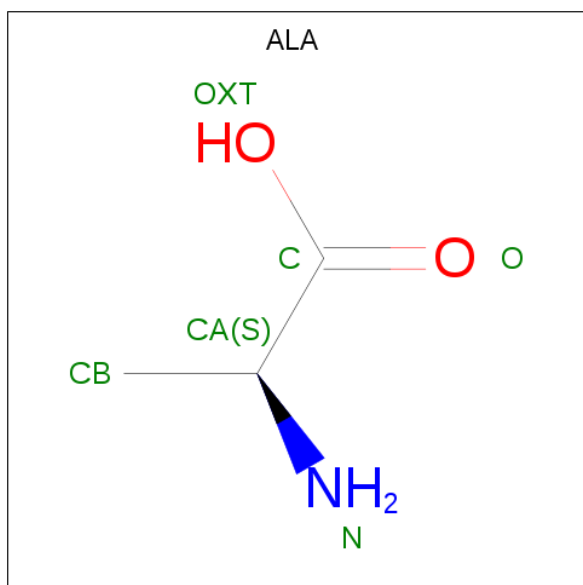
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is PROLINE (three-letter code: PRO) (formula: C₅H₉NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	5	1	2		
5	B	1	Total	C	N	O	0	0
			8	5	1	2		
5	C	1	Total	C	N	O	0	0
			8	5	1	2		
5	D	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 6 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			6	3	1	2		
6	B	1	Total	C	N	O	0	0
			5	3	1	1		

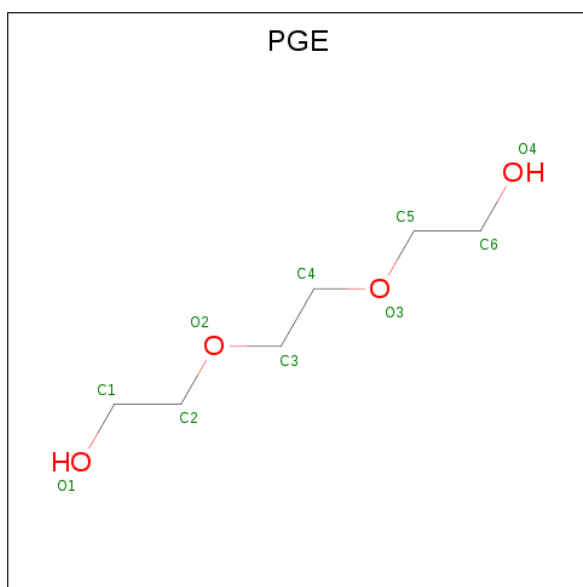
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	1	Total	Ca	0	0
			1	1		
7	C	2	Total	Ca	0	0
			2	2		

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

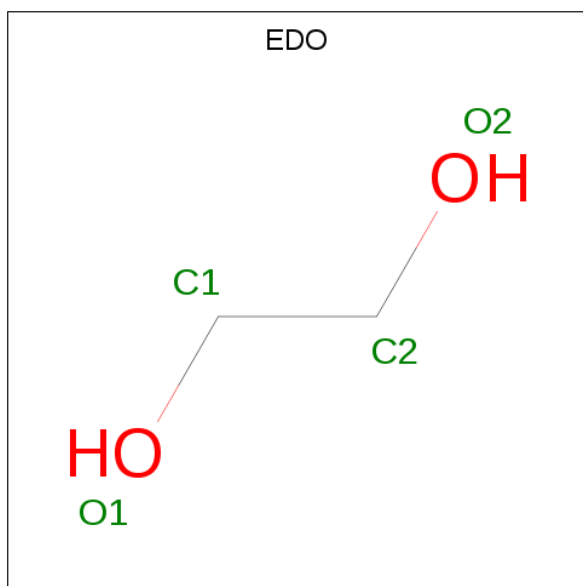
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	3	Total	Mn	0	0
			3	3		
8	A	3	Total	Mn	0	0
			3	3		
8	D	3	Total	Mn	0	0
			3	3		
8	C	3	Total	Mn	0	0
			3	3		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

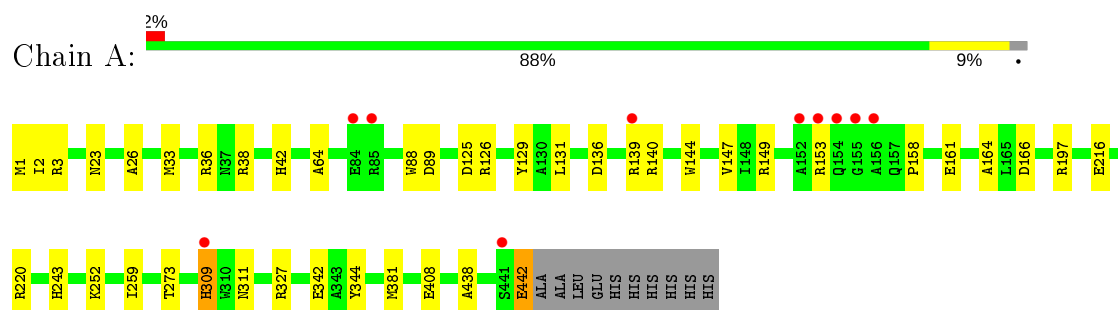
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	303	Total	O	0	0
			303	303		
11	B	275	Total	O	0	0
			275	275		
11	C	268	Total	O	0	0
			268	268		
11	D	306	Total	O	0	0
			306	306		

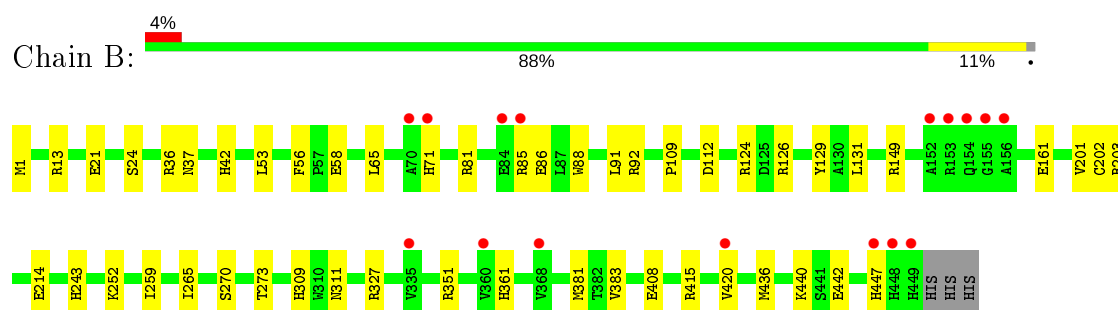
3 Residue-property plots [i](#)

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.

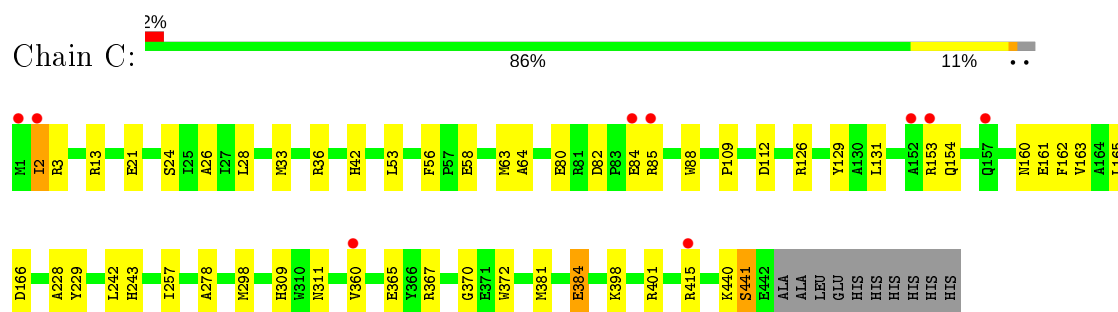
• Molecule 1: Aminopeptidase P



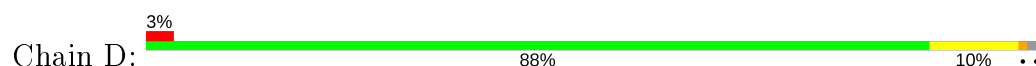
• Molecule 1: Aminopeptidase P

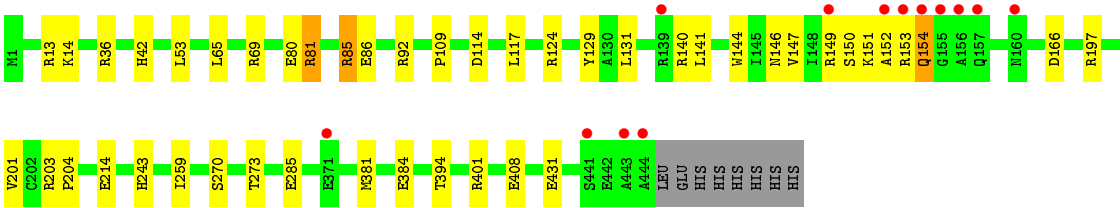


• Molecule 1: Aminopeptidase P



• Molecule 1: Aminopeptidase P





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.20 Å 123.43 Å 149.49 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.01 – 1.78 48.01 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.01-1.78) 99.4 (48.01-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.78 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.210 , 0.221 0.210 , 0.221	Depositor DCC
R_{free} test set	2000 reflections (1.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15378	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PGE, NA, CA, MN, EDO, SO4

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	0.55	0/3603	0.64	2/4880 (0.0%)
1	B	0.53	1/3642 (0.0%)	0.59	0/4937
1	C	0.54	1/3624 (0.0%)	0.59	0/4911
1	D	0.56	1/3597 (0.0%)	0.62	1/4875 (0.0%)
All	All	0.54	3/14466 (0.0%)	0.61	3/19603 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	384	GLU	CD-OE1	-5.54	1.19	1.25
1	D	270	SER	CB-OG	-5.37	1.35	1.42
1	B	270	SER	CB-OG	-5.15	1.35	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	81	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	A	327	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	A	89	ASP	N-CA-C	5.33	125.38	111.00

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	3511	0	3442	35	1
1	B	3550	0	3478	39	0
1	C	3523	0	3471	49	1
1	D	3509	0	3441	29	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
3	A	6	0	8	2	0
3	D	18	0	24	4	0
4	A	5	0	0	1	0
4	D	10	0	0	0	0
5	A	8	0	7	3	0
5	B	8	0	7	1	0
5	C	8	0	7	1	0
5	D	8	0	7	0	0
6	A	6	0	4	0	0
6	B	5	0	4	1	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
8	A	3	0	0	0	0
8	B	3	0	0	0	0
8	C	3	0	0	0	0
8	D	3	0	0	0	0
9	B	10	0	14	5	0
10	B	8	0	12	7	0
10	C	8	0	12	2	0
10	D	4	0	6	0	0
11	A	303	0	0	6	0
11	B	275	0	0	3	0
11	C	268	0	0	16	0
11	D	306	0	0	4	0
All	All	15378	0	13944	149	1

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 (149) 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:C:33:MET:HE3	11:C:826:HOH:O	1.27	1.33
1:B:243:HIS:NE2	5:B:506:PRO:HD2	1.82	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HH12	3:A:502:GOL:H31	1.30	0.93
1:C:160:ASN:HB3	11:C:818:HOH:O	1.71	0.90
1:C:440:LYS:HE2	11:C:798:HOH:O	1.76	0.85
1:A:309[A]:HIS:HD2	1:A:311:ASN:H	1.25	0.84
1:D:201[B]:VAL:HG11	1:D:214:GLU:HG3	1.60	0.83
5:A:504:PRO:OXT	1:C:88:TRP:HZ3	1.61	0.81
1:C:367:ARG:NH2	1:C:370:GLY:O	2.15	0.80
1:B:327:ARG:NH1	11:B:601:HOH:O	2.14	0.80
1:B:203:ARG:HB3	9:B:503:PGE:H3	1.62	0.79
1:C:28[B]:LEU:HD22	11:C:856:HOH:O	1.81	0.79
1:A:438:ALA:O	1:A:442:GLU:HG2	1.82	0.79
1:C:309[A]:HIS:HE1	1:C:311:ASN:HB3	1.49	0.78
1:A:33[B]:MET:CE	11:A:781:HOH:O	2.37	0.71
1:B:243:HIS:CE1	10:B:505:EDO:H21	2.25	0.71
1:C:154:GLN:OE1	1:C:154:GLN:N	2.24	0.71
1:A:140[B]:ARG:NH2	11:A:602:HOH:O	2.24	0.70
1:B:252:LYS:HE2	11:B:621:HOH:O	1.92	0.69
1:A:38:ARG:NH1	3:A:502:GOL:H31	2.07	0.68
1:C:82:ASP:OD2	1:C:85:ARG:HD3	1.95	0.67
1:A:136:ASP:OD1	1:A:139:ARG:NH1	2.26	0.67
1:B:201[A]:VAL:HG11	1:B:214:GLU:HG3	1.76	0.67
1:A:33[B]:MET:HE3	11:A:781:HOH:O	1.95	0.66
1:C:2:ILE:HD12	1:C:3:ARG:H	1.63	0.64
1:B:129:TYR:CZ	1:B:131:LEU:HD13	2.32	0.64
1:D:203:ARG:NH2	11:D:605:HOH:O	2.30	0.63
1:C:33:MET:HB3	11:C:826:HOH:O	1.98	0.63
5:A:504:PRO:OXT	1:C:88:TRP:CZ3	2.50	0.62
1:C:28[A]:LEU:HD12	11:C:856:HOH:O	1.99	0.62
1:C:372:TRP:CD1	10:C:503:EDO:H21	2.34	0.62
1:A:309[A]:HIS:CD2	1:A:311:ASN:H	2.13	0.61
1:A:88:TRP:O	1:C:243:HIS:HB2	2.01	0.60
1:B:126:ARG:HG2	1:B:161:GLU:HB2	1.84	0.60
1:D:203:ARG:NH1	1:D:204:PRO:O	2.35	0.60
1:D:36:ARG:HG3	1:D:42:HIS:CE1	2.37	0.59
1:C:298:MET:HE1	11:C:865:HOH:O	2.02	0.59
1:C:229:TYR:HD1	1:C:360[A]:VAL:HG11	1.69	0.58
1:D:69:ARG:HA	3:D:501:GOL:H11	1.85	0.58
1:C:33:MET:CG	11:C:826:HOH:O	2.52	0.58
1:A:126:ARG:HG2	1:A:161:GLU:HB2	1.86	0.57
1:C:28[B]:LEU:HD21	1:C:165:LEU:HD23	1.86	0.57
1:B:85:ARG:HG2	1:B:92:ARG:NH2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360[B]:VAL:HG23	11:C:777:HOH:O	2.05	0.56
1:C:441:SER:OG	11:C:601:HOH:O	2.00	0.56
1:B:21:GLU:HG3	1:B:126:ARG:NH1	2.21	0.56
1:B:21:GLU:O	1:B:24:SER:OG	2.21	0.56
1:B:436:MET:HB3	9:B:503:PGE:H62	1.87	0.56
1:A:252:LYS:HE2	11:A:611:HOH:O	2.06	0.56
1:B:361:HIS:HE1	10:B:505:EDO:H22	1.71	0.56
1:A:220:ARG:HD3	11:C:729:HOH:O	2.06	0.56
1:C:80:GLU:HG3	1:C:109:PRO:HB3	1.89	0.55
1:D:401:ARG:HH22	3:D:503:GOL:H2	1.72	0.54
1:B:243:HIS:HE1	10:B:505:EDO:H21	1.70	0.54
1:C:126:ARG:HD3	1:C:163:VAL:HG21	1.88	0.54
1:C:242:LEU:O	11:C:602:HOH:O	2.18	0.54
1:A:309[A]:HIS:HD2	1:A:311:ASN:N	2.01	0.54
1:B:81:ARG:NH1	1:B:86:GLU:OE1	2.42	0.53
1:D:85:ARG:HD3	1:D:92:ARG:NH2	2.23	0.53
1:B:415:ARG:HG2	1:B:415:ARG:HH21	1.72	0.53
1:C:33:MET:HG2	11:C:826:HOH:O	2.08	0.53
1:C:309[A]:HIS:CE1	1:C:311:ASN:HB3	2.37	0.52
1:A:36:ARG:HG3	1:A:42:HIS:CE1	2.44	0.52
1:B:351:ARG:HG3	6:B:507:ALA:HB3	1.92	0.52
1:D:151:LYS:O	1:D:152:ALA:C	2.48	0.52
1:A:216:GLU:O	1:A:220:ARG:HG3	2.10	0.52
1:A:129:TYR:CZ	1:A:131:LEU:HD13	2.45	0.51
1:B:1:MET:HE2	1:B:265:ILE:HG23	1.91	0.51
1:B:36:ARG:HD2	1:B:37:ASN:OD1	2.11	0.51
1:C:28[A]:LEU:HB2	1:C:63:MET:HG2	1.92	0.51
1:B:13:ARG:HG2	1:B:65:LEU:HD21	1.92	0.51
1:D:166:ASP:HB2	11:D:692:HOH:O	2.10	0.50
1:A:243:HIS:HE2	5:A:504:PRO:N	2.07	0.50
1:D:151:LYS:O	1:D:154:GLN:N	2.44	0.50
1:D:285:GLU:H	1:D:285:GLU:CD	2.14	0.50
1:A:131:LEU:HD23	1:A:164:ALA:HA	1.93	0.50
1:B:383:VAL:O	1:B:408:GLU:HA	2.11	0.50
1:C:28[A]:LEU:HD11	1:C:165:LEU:HD23	1.93	0.49
1:C:398:LYS:HG2	1:C:401:ARG:CZ	2.43	0.49
1:B:243:HIS:HE1	10:B:505:EDO:C2	2.25	0.48
1:C:372:TRP:HD1	10:C:503:EDO:H21	1.78	0.48
1:C:84:GLU:HB2	11:C:704:HOH:O	2.12	0.48
1:C:56:PHE:CE2	1:C:58:GLU:HB2	2.48	0.48
1:A:252:LYS:NZ	11:A:611:HOH:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ARG:HH22	10:B:504:EDO:H22	1.77	0.48
1:D:431:GLU:OE1	11:D:601:HOH:O	2.19	0.48
1:D:147:VAL:O	1:D:150:SER:OG	2.30	0.48
1:A:3:ARG:NH2	4:A:503:SO4:O1	2.47	0.47
1:B:124:ARG:NH1	11:B:610:HOH:O	2.47	0.47
1:B:71:HIS:ND1	1:B:71:HIS:O	2.43	0.47
1:D:114:ASP:CG	1:D:140:ARG:HH22	2.17	0.47
1:C:80:GLU:CG	1:C:109:PRO:HB3	2.44	0.47
1:A:88:TRP:O	1:C:243:HIS:N	2.45	0.47
1:D:124:ARG:HH22	3:D:501:GOL:H31	1.80	0.47
1:B:309:HIS:HE1	1:B:311:ASN:HB3	1.80	0.47
1:C:36:ARG:HG3	1:C:42:HIS:NE2	2.30	0.47
1:D:13:ARG:HD3	1:D:53:LEU:O	2.14	0.47
1:B:88:TRP:O	1:D:243:HIS:HB2	2.14	0.46
1:C:160:ASN:OD1	1:C:160:ASN:N	2.41	0.46
1:D:141:LEU:HA	1:D:144:TRP:CE3	2.51	0.46
1:A:144:TRP:O	1:A:147:VAL:HG22	2.16	0.46
1:A:273:THR:H	1:A:408:GLU:HB3	1.81	0.46
1:C:21:GLU:HG3	1:C:126:ARG:CZ	2.46	0.45
1:C:228:ALA:HB1	1:C:360[A]:VAL:CG1	2.47	0.45
1:B:243:HIS:CE1	10:B:505:EDO:C2	2.98	0.44
1:D:384:GLU:HB3	1:D:408:GLU:HB2	1.98	0.44
1:C:129:TYR:CZ	1:C:131:LEU:HG	2.52	0.44
1:B:124:ARG:HH22	10:B:504:EDO:C2	2.30	0.44
1:D:401:ARG:HH12	3:D:503:GOL:H2	1.82	0.44
1:B:36:ARG:HG3	1:B:42:HIS:CE1	2.53	0.44
1:B:13:ARG:HD3	1:B:53:LEU:O	2.18	0.44
1:A:252:LYS:CE	11:A:611:HOH:O	2.65	0.43
1:D:146:ASN:HA	1:D:149:ARG:HG3	2.00	0.43
1:C:28[B]:LEU:CD2	11:C:856:HOH:O	2.53	0.43
1:B:109:PRO:HG2	1:B:112:ASP:OD2	2.18	0.43
1:D:114:ASP:OD1	1:D:140:ARG:NH2	2.47	0.43
1:B:1:MET:CE	1:B:265:ILE:HG23	2.49	0.43
1:B:440:LYS:HG3	9:B:503:PGE:H22	2.00	0.43
1:A:149:ARG:HG2	1:A:158:PRO:HG3	2.00	0.43
1:B:440:LYS:HB2	9:B:503:PGE:H52	2.01	0.43
1:C:384:GLU:OE1	5:C:504:PRO:HA	2.19	0.42
1:C:13:ARG:HD3	1:C:53:LEU:O	2.19	0.42
1:D:13:ARG:HG2	1:D:65:LEU:HD21	2.00	0.42
1:C:21:GLU:O	1:C:24:SER:OG	2.21	0.42
1:A:342:GLU:HA	1:A:344:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:LYS:NZ	11:D:606:HOH:O	2.32	0.42
1:C:257:ILE:CD1	1:C:278:ALA:HB2	2.51	0.41
1:D:117:LEU:HD23	1:D:144:TRP:CZ3	2.55	0.41
1:A:1:MET:HG2	1:A:2:ILE:H	1.84	0.41
1:C:398:LYS:HG3	11:C:771:HOH:O	2.19	0.41
1:D:129:TYR:CZ	1:D:131:LEU:HG	2.56	0.41
1:C:228:ALA:HB1	1:C:360[B]:VAL:HG22	2.02	0.41
1:D:81:ARG:HD2	1:D:86:GLU:OE2	2.20	0.41
1:B:202:CYS:O	9:B:503:PGE:O4	2.39	0.41
1:A:140[B]:ARG:HD2	1:A:144:TRP:CZ2	2.56	0.41
1:A:259:ILE:O	1:A:273:THR:HA	2.21	0.41
1:C:109:PRO:HG2	1:C:112:ASP:OD2	2.21	0.41
1:C:161:GLU:O	1:C:162:PHE:HD1	2.04	0.41
1:B:56:PHE:CE2	1:B:58:GLU:HB2	2.55	0.41
1:C:26:ALA:O	1:C:64:ALA:HA	2.21	0.41
1:A:23:ASN:ND2	1:A:125:ASP:OD1	2.50	0.40
1:A:197:ARG:HD2	1:A:197:ARG:HA	1.94	0.40
1:D:80:GLU:HG3	1:D:109:PRO:HB3	2.03	0.40
1:A:26:ALA:O	1:A:64:ALA:HA	2.22	0.40
1:A:140[A]:ARG:HG2	1:A:144:TRP:CZ2	2.56	0.40
1:B:259:ILE:O	1:B:273:THR:HA	2.21	0.40
1:D:259:ILE:O	1:D:273:THR:HA	2.21	0.40
1:B:442:GLU:OE1	1:B:447:HIS:ND1	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASP:OD2	1:C:415:ARG:NH2[2_354]	2.03	0.17

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	444/452 (98%)	436 (98%)	8 (2%)	0	100	100
1	B	451/452 (100%)	445 (99%)	6 (1%)	0	100	100
1	C	447/452 (99%)	441 (99%)	6 (1%)	0	100	100
1	D	445/452 (98%)	438 (98%)	7 (2%)	0	100	100
All	All	1787/1808 (99%)	1760 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	355/359 (99%)	349 (98%)	6 (2%)	60	48
1	B	358/359 (100%)	353 (99%)	5 (1%)	67	56
1	C	357/359 (99%)	351 (98%)	6 (2%)	60	48
1	D	354/359 (99%)	348 (98%)	6 (2%)	60	48
All	All	1424/1436 (99%)	1401 (98%)	23 (2%)	62	51

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ARG
1	A	166	ASP
1	A	309[A]	HIS
1	A	309[B]	HIS
1	A	381	MET
1	A	442	GLU
1	B	91	LEU
1	B	149	ARG
1	B	381	MET
1	B	420[A]	VAL
1	B	420[B]	VAL
1	C	2	ILE
1	C	153	ARG

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Mol	Chain	Res	Type
1	C	166	ASP
1	C	365	GLU
1	C	381	MET
1	C	441	SER
1	D	85	ARG
1	D	153	ARG
1	D	154	GLN
1	D	197	ARG
1	D	381	MET
1	D	394	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	B	243	HIS
1	C	42	HIS
1	D	361	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 21 are monoatomic - leaving 19 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	$\# Z > 2$
10	EDO	D	506	-	3,3,3	0.30	0	2,2,2	0.35	0
6	ALA	B	507	-	3,4,5	0.75	0	2,4,6	0.83	0
9	PGE	B	503	2	9,9,9	0.27	0	8,8,8	0.93	0
5	PRO	B	506	-	5,8,8	1.72	1 (20%)	6,10,10	0.91	0
5	PRO	C	504	-	5,8,8	1.75	1 (20%)	6,10,10	1.01	0
10	EDO	C	503	-	3,3,3	0.46	0	2,2,2	0.27	0
4	SO4	A	503	-	4,4,4	0.26	0	6,6,6	0.15	0
3	GOL	A	502	-	5,5,5	0.66	0	5,5,5	0.48	0
10	EDO	B	505	-	3,3,3	0.44	0	2,2,2	0.28	0
4	SO4	D	505	-	4,4,4	0.37	0	6,6,6	0.36	0
10	EDO	B	504	-	3,3,3	0.53	0	2,2,2	0.37	0
3	GOL	D	503	-	5,5,5	0.33	0	5,5,5	0.47	0
5	PRO	D	510	-	5,8,8	2.12	1 (20%)	6,10,10	0.95	0
10	EDO	C	502	-	3,3,3	0.38	0	2,2,2	0.79	0
5	PRO	A	504	-	5,8,8	0.72	0	6,10,10	1.06	1 (16%)
4	SO4	D	504	-	4,4,4	0.36	0	6,6,6	0.30	0
6	ALA	A	505	-	2,5,5	0.76	0	2,6,6	0.02	0
3	GOL	D	502	-	5,5,5	0.48	0	5,5,5	0.71	0
3	GOL	D	501	-	5,5,5	0.33	0	5,5,5	0.62	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
6	ALA	B	507	-	-	0/0/2/4	-
9	PGE	B	503	2	-	4/7/7/7	-
5	PRO	B	506	-	-	0/0/11/11	0/1/1/1
5	PRO	C	504	-	-	0/0/11/11	0/1/1/1
10	EDO	C	503	-	-	0/1/1/1	-
6	ALA	A	505	-	-	0/0/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-
10	EDO	B	505	-	-	1/1/1/1	-
10	EDO	D	506	-	-	0/1/1/1	-
10	EDO	B	504	-	-	1/1/1/1	-
3	GOL	D	503	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PRO	D	510	-	-	0/0/11/11	0/1/1/1
10	EDO	C	502	-	-	1/1/1/1	-
5	PRO	A	504	-	-	0/0/11/11	0/1/1/1
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	D	501	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	510	PRO	CB-CA	-4.61	1.48	1.54
5	C	504	PRO	CB-CA	-3.60	1.50	1.54
5	B	506	PRO	CB-CA	-3.56	1.50	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	PRO	CD-N-CA	2.07	112.61	107.06

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	GOL	O1-C1-C2-C3
3	A	502	GOL	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-C3
3	D	502	GOL	O1-C1-C2-O2
3	A	502	GOL	O2-C2-C3-O3
9	B	503	PGE	O3-C5-C6-O4
3	A	502	GOL	C1-C2-C3-O3
9	B	503	PGE	O2-C3-C4-O3
9	B	503	PGE	C3-C4-O3-C5
10	B	505	EDO	O1-C1-C2-O2
10	C	502	EDO	O1-C1-C2-O2
9	B	503	PGE	C6-C5-O3-C4
10	B	504	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	507	ALA	1	0
9	B	503	PGE	5	0
5	B	506	PRO	1	0
5	C	504	PRO	1	0
10	C	503	EDO	2	0
4	A	503	SO4	1	0
3	A	502	GOL	2	0
10	B	505	EDO	5	0
10	B	504	EDO	2	0
3	D	503	GOL	2	0
5	A	504	PRO	3	0
3	D	501	GOL	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	442/452 (97%)	-0.01	10 (2%) 60 60	12, 21, 49, 93	0
1	B	449/452 (99%)	0.14	16 (3%) 42 41	12, 24, 54, 86	1 (0%)
1	C	442/452 (97%)	-0.04	9 (2%) 65 65	14, 24, 53, 82	0
1	D	444/452 (98%)	0.09	13 (2%) 51 50	12, 23, 54, 101	0
All	All	1777/1808 (98%)	0.05	48 (2%) 54 53	12, 23, 53, 101	1 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	420[A]	VAL	7.7
1	A	153	ARG	5.7
1	A	152	ALA	5.0
1	C	1	MET	3.9
1	D	155	GLY	3.9
1	B	70	ALA	3.8
1	C	360[A]	VAL	3.8
1	D	152	ALA	3.8
1	B	153	ARG	3.7
1	C	415	ARG	3.7
1	D	153	ARG	3.6
1	B	449	HIS	3.6
1	A	309[A]	HIS	3.5
1	A	155	GLY	3.4
1	A	85	ARG	3.1
1	A	154	GLN	3.1
1	C	153	ARG	2.9
1	D	154	GLN	2.9
1	B	447	HIS	2.9
1	D	139	ARG	2.8
1	B	360[A]	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	84	GLU	2.7
1	B	84	GLU	2.7
1	A	156	ALA	2.6
1	A	441	SER	2.6
1	A	84	GLU	2.6
1	D	371	GLU	2.6
1	D	149	ARG	2.6
1	C	152	ALA	2.6
1	D	157	GLN	2.6
1	B	448	HIS	2.5
1	B	152	ALA	2.5
1	B	85	ARG	2.5
1	B	71	HIS	2.5
1	D	156	ALA	2.4
1	D	444	ALA	2.4
1	B	156	ALA	2.3
1	C	85	ARG	2.3
1	D	160	ASN	2.3
1	D	441	SER	2.2
1	C	157	GLN	2.2
1	A	139	ARG	2.2
1	B	335	VAL	2.2
1	C	2	ILE	2.2
1	D	443	ALA	2.1
1	B	368	VAL	2.1
1	B	154	GLN	2.1
1	B	155	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PRO	A	504	8/8	0.56	0.27	27,30,43,43	0
10	EDO	B	505	4/4	0.65	0.30	40,44,46,48	0
5	PRO	B	506	8/8	0.71	0.26	30,37,48,50	0
5	PRO	C	504	8/8	0.71	0.23	28,38,50,53	0
9	PGE	B	503	10/10	0.71	0.36	17,27,34,36	10
10	EDO	C	503	4/4	0.74	0.15	44,47,47,51	0
7	CA	A	506	1/1	0.74	0.11	64,64,64,64	0
7	CA	B	509	1/1	0.74	0.11	76,76,76,76	0
5	PRO	D	510	8/8	0.76	0.22	28,38,50,53	0
3	GOL	D	501	6/6	0.80	0.19	40,42,45,47	0
6	ALA	A	505	6/6	0.81	0.28	40,46,47,48	0
3	GOL	D	503	6/6	0.81	0.31	42,44,46,47	0
10	EDO	C	502	4/4	0.85	0.20	33,42,45,49	0
10	EDO	B	504	4/4	0.86	0.10	45,45,46,47	0
3	GOL	A	502	6/6	0.86	0.17	31,36,39,50	0
6	ALA	B	507	5/6	0.86	0.20	34,37,40,44	0
10	EDO	D	506	4/4	0.86	0.17	38,39,43,45	0
7	CA	B	508	1/1	0.89	0.04	80,80,80,80	0
8	MN	B	510	1/1	0.89	0.12	28,28,28,28	1
2	NA	C	501	1/1	0.90	0.10	36,36,36,36	0
7	CA	C	506	1/1	0.91	0.08	48,48,48,48	0
3	GOL	D	502	6/6	0.92	0.14	27,38,39,40	0
8	MN	A	507	1/1	0.93	0.18	28,28,28,28	1
7	CA	C	505	1/1	0.94	0.06	56,56,56,56	0
2	NA	A	501	1/1	0.95	0.08	32,32,32,32	0
8	MN	C	508	1/1	0.96	0.13	28,28,28,28	1
4	SO4	A	503	5/5	0.96	0.15	24,26,31,33	5
8	MN	A	509	1/1	0.97	0.14	31,31,31,31	0
8	MN	A	508	1/1	0.97	0.07	28,28,28,28	0
2	NA	B	501	1/1	0.97	0.17	34,34,34,34	0
8	MN	D	507	1/1	0.97	0.10	37,37,37,37	0
8	MN	B	511	1/1	0.97	0.08	28,28,28,28	0
8	MN	D	509	1/1	0.97	0.12	28,28,28,28	1
4	SO4	D	505	5/5	0.98	0.10	23,26,30,32	5
8	MN	B	512	1/1	0.98	0.11	33,33,33,33	0
4	SO4	D	504	5/5	0.98	0.08	19,21,23,27	0
8	MN	D	508	1/1	0.98	0.07	28,28,28,28	0
2	NA	B	502	1/1	0.98	0.24	32,32,32,32	0
8	MN	C	507	1/1	0.99	0.03	37,37,37,37	0
8	MN	C	509	1/1	1.00	0.04	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.