



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:32 PM UTC

PDB ID : 4ZE8 / pdb_00004ze8
Title : PBP AccA from *A. tumefaciens* C58
Authors : El Sahili, A.; Morera, S.
Deposited on : 2015-04-20
Resolution : 1.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

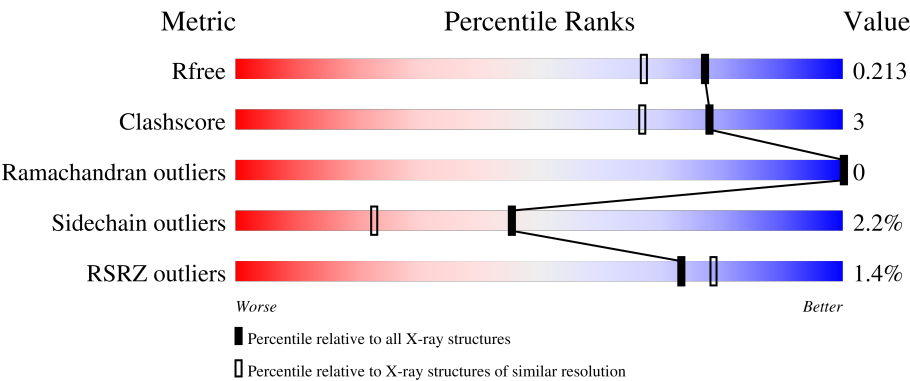
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	499	% 90%8%..
1	B	499	% 90%8%..
1	C	499	2% 89%8%..
1	D	499	% 89%9%..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17887 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 ABC transporter, substrate binding protein (Agrocinopines A and B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	5	0
			3988	2572	669	727	20			
1	B	491	Total	C	N	O	S	0	4	0
			3978	2565	666	728	19			
1	C	491	Total	C	N	O	S	0	6	0
			3991	2574	669	728	20			
1	D	491	Total	C	N	O	S	0	1	0
			3957	2550	663	725	19			

There are 28 discrepancies between the modelled and reference sequences:

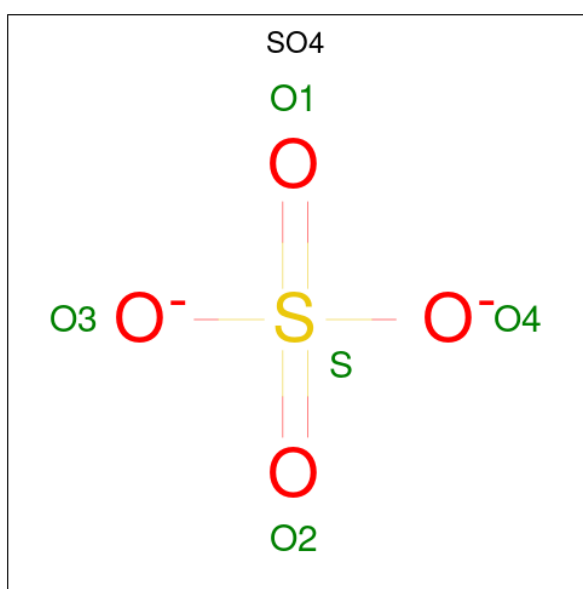
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MET	-	initiating methionine	UNP Q7D2F4
A	522	HIS	-	expression tag	UNP Q7D2F4
A	523	HIS	-	expression tag	UNP Q7D2F4
A	524	HIS	-	expression tag	UNP Q7D2F4
A	525	HIS	-	expression tag	UNP Q7D2F4
A	526	HIS	-	expression tag	UNP Q7D2F4
A	527	HIS	-	expression tag	UNP Q7D2F4
B	29	MET	-	initiating methionine	UNP Q7D2F4
B	522	HIS	-	expression tag	UNP Q7D2F4
B	523	HIS	-	expression tag	UNP Q7D2F4
B	524	HIS	-	expression tag	UNP Q7D2F4
B	525	HIS	-	expression tag	UNP Q7D2F4
B	526	HIS	-	expression tag	UNP Q7D2F4
B	527	HIS	-	expression tag	UNP Q7D2F4
C	29	MET	-	initiating methionine	UNP Q7D2F4
C	522	HIS	-	expression tag	UNP Q7D2F4
C	523	HIS	-	expression tag	UNP Q7D2F4
C	524	HIS	-	expression tag	UNP Q7D2F4
C	525	HIS	-	expression tag	UNP Q7D2F4
C	526	HIS	-	expression tag	UNP Q7D2F4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	527	HIS	-	expression tag	UNP Q7D2F4
D	29	MET	-	initiating methionine	UNP Q7D2F4
D	522	HIS	-	expression tag	UNP Q7D2F4
D	523	HIS	-	expression tag	UNP Q7D2F4
D	524	HIS	-	expression tag	UNP Q7D2F4
D	525	HIS	-	expression tag	UNP Q7D2F4
D	526	HIS	-	expression tag	UNP Q7D2F4
D	527	HIS	-	expression tag	UNP Q7D2F4

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

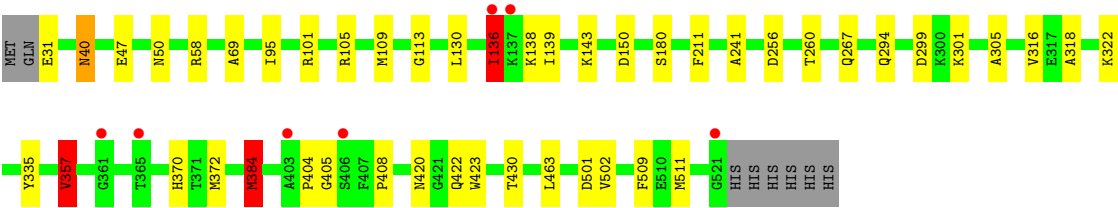
- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	506	Total 506	O 506	0	0
6	B	430	Total 430	O 430	0	0
6	C	504	Total 504	O 504	0	0
6	D	452	Total 452	O 452	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.95Å 179.35Å 81.60Å 90.00° 93.51° 90.00°	Depositor
Resolution (Å)	40.88 – 1.72 40.88 – 1.72	Depositor EDS
% Data completeness (in resolution range)	97.3 (40.88-1.72) 97.3 (40.88-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 1.72Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.166 , 0.197 0.181 , 0.213	Depositor DCC
R_{free} test set	10754 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.818	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.0	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	17887	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 33.94 % 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 7.3868e-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: EDO, GOL, SO4, PEG

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	0.82	2/4108 (0.0%)	1.07	11/5579 (0.2%)
1	B	0.80	1/4095 (0.0%)	1.08	9/5563 (0.2%)
1	C	0.83	2/4114 (0.0%)	1.07	12/5587 (0.2%)
1	D	0.79	1/4069 (0.0%)	1.08	12/5526 (0.2%)
All	All	0.81	6/16386 (0.0%)	1.07	44/22255 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	384	MET	SD-CE	-9.95	1.54	1.79
1	A	384	MET	SD-CE	-8.61	1.58	1.79
1	C	109	MET	SD-CE	-6.39	1.63	1.79
1	A	109	MET	SD-CE	-5.79	1.65	1.79
1	D	384	MET	SD-CE	-5.63	1.65	1.79
1	B	109	MET	SD-CE	-5.60	1.65	1.79

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	357	VAL	N-CA-CB	7.60	120.88	110.54
1	A	357	VAL	N-CA-CB	7.37	119.18	110.55
1	A	501	ASP	CA-CB-CG	7.25	119.85	112.60
1	C	423	TRP	N-CA-C	7.05	121.73	113.20
1	D	241	ALA	N-CA-C	7.05	118.96	111.28
1	C	47	GLU	N-CA-C	-6.82	99.47	109.50
1	D	423	TRP	N-CA-C	6.77	121.40	113.20
1	B	47	GLU	N-CA-C	-6.72	99.62	109.50
1	D	180	SER	N-CA-C	6.51	120.54	112.59
1	A	241	ALA	N-CA-C	6.46	119.14	111.33
1	B	241	ALA	N-CA-C	6.27	118.64	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	ALA	N-CA-C	6.27	118.92	111.33
1	B	423	TRP	N-CA-C	6.21	120.71	113.20
1	B	211	PHE	CA-CB-CG	6.07	119.87	113.80
1	A	180	SER	N-CA-C	6.04	119.96	112.59
1	C	180[A]	SER	N-CA-C	5.92	119.81	112.59
1	C	180[B]	SER	N-CA-C	5.92	119.81	112.59
1	A	423	TRP	N-CA-C	5.90	120.34	113.20
1	D	501	ASP	CA-CB-CG	5.81	118.41	112.60
1	D	130	LEU	N-CA-C	5.77	120.04	112.13
1	B	130	LEU	N-CA-C	5.76	119.78	111.02
1	B	501	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	130	LEU	N-CA-C	5.72	119.72	111.02
1	C	136	ILE	N-CA-C	5.72	117.14	110.62
1	D	136	ILE	N-CA-C	5.68	118.15	111.05
1	B	136	ILE	N-CA-C	5.68	117.09	110.62
1	A	211	PHE	CA-CB-CG	5.66	119.46	113.80
1	D	211	PHE	CA-CB-CG	5.53	119.33	113.80
1	A	136	ILE	N-CA-C	5.52	116.91	110.62
1	C	150	ASP	N-CA-C	-5.49	102.08	110.14
1	A	150	ASP	N-CA-C	-5.46	102.11	110.14
1	B	150	ASP	N-CA-C	-5.42	102.18	110.14
1	D	47	GLU	N-CA-C	-5.39	100.15	109.58
1	C	425	THR	N-CA-C	-5.36	104.09	111.81
1	C	420	ASN	CA-CB-CG	5.34	117.94	112.60
1	D	150	ASP	N-CA-C	-5.31	102.34	110.14
1	B	97	GLU	CB-CG-CD	5.27	121.56	112.60
1	A	47	GLU	N-CA-C	-5.23	99.98	109.44
1	D	420	ASN	CA-CB-CG	5.22	117.82	112.60
1	D	357	VAL	N-CA-CB	5.21	118.39	110.58
1	A	130	LEU	N-CA-C	5.17	119.21	112.13
1	C	224	ALA	N-CA-C	-5.13	106.87	113.02
1	D	301	LYS	N-CA-C	5.12	117.27	111.02
1	A	455	GLU	CB-CG-CD	5.01	121.11	112.60

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	3988	0	3932	23	0
1	B	3978	0	3915	18	0
1	C	3991	0	3937	25	0
1	D	3957	0	3897	26	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	8	0	12	0	0
3	B	12	0	18	0	0
3	C	8	0	12	1	0
3	D	4	0	6	0	0
4	A	7	0	10	0	0
5	A	6	0	8	3	0
5	D	6	0	8	1	0
6	A	506	0	0	4	0
6	B	430	0	0	2	0
6	C	504	0	0	6	0
6	D	452	0	0	2	0
All	All	17887	0	15755	88	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 3.

All (88) 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)
3:C:603:EDO:H22	6:C:862:HOH:O	1.68	0.92
6:A:1147:HOH:O	1:B:365:THR:HG22	1.78	0.80
1:C:40:ASN:HD22	1:C:40:ASN:H	1.38	0.71
1:A:40:ASN:HD22	1:A:40:ASN:H	1.38	0.69
1:B:40:ASN:H	1:B:40:ASN:HD22	1.40	0.68
1:D:40:ASN:HD22	1:D:40:ASN:H	1.41	0.67
1:D:136:ILE:HD11	1:D:143:LYS:H	1.61	0.66
1:A:370:HIS:HD2	6:A:785:HOH:O	1.81	0.64
1:C:247:VAL:HG13	1:C:269:ILE:HD11	1.81	0.63
1:A:109:MET:HE1	1:C:458:GLN:NE2	2.17	0.60
1:D:509:PHE:HD2	1:D:511:MET:HG2	1.69	0.57
1:B:370:HIS:HD2	6:B:753:HOH:O	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ASN:HD21	1:C:58:ARG:HH12	1.54	0.55
1:C:509:PHE:HD2	1:C:511:MET:HG2	1.72	0.55
1:D:40:ASN:HD21	1:D:58:ARG:HH12	1.55	0.55
1:C:286:HIS:HD2	6:C:888:HOH:O	1.90	0.54
1:D:50:ASN:HD21	1:D:139:ILE:HA	1.72	0.54
1:B:509:PHE:HD2	1:B:511:MET:HG2	1.72	0.54
1:D:422:GLN:HE22	1:D:430:THR:H	1.56	0.53
1:A:440:GLN:NE2	6:A:701:HOH:O	2.41	0.53
1:C:40:ASN:ND2	1:C:58:ARG:HH12	2.07	0.53
1:A:40:ASN:HD21	1:A:58:ARG:HH12	1.56	0.53
1:A:509:PHE:HD2	1:A:511:MET:HG2	1.73	0.53
1:D:40:ASN:ND2	1:D:58:ARG:HH12	2.07	0.53
1:B:40:ASN:HD21	1:B:58:ARG:HH12	1.56	0.52
1:C:503:HIS:HD2	6:C:1119:HOH:O	1.92	0.52
1:A:109:MET:HE3	1:A:113:GLY:HA2	1.90	0.52
1:A:372:MET:HE3	1:A:404:PRO:HG3	1.92	0.52
1:A:422:GLN:HE22	1:A:430:THR:H	1.56	0.52
1:D:95:ILE:HD11	1:D:101:ARG:HB2	1.91	0.52
1:C:422:GLN:HE22	1:C:430:THR:H	1.56	0.52
1:B:422:GLN:HE22	1:B:430:THR:H	1.57	0.51
1:A:418:TRP:CE2	5:A:606:GOL:H12	2.46	0.51
1:A:40:ASN:ND2	1:A:58:ARG:HH12	2.08	0.51
1:C:109:MET:HE3	1:C:113:GLY:HA2	1.93	0.51
1:B:40:ASN:ND2	1:B:58:ARG:HH12	2.09	0.51
1:B:109:MET:HE3	1:B:113:GLY:HA2	1.93	0.50
1:D:370:HIS:HD2	6:D:819:HOH:O	1.94	0.49
1:A:416:ARG:HE	5:A:606:GOL:C1	2.24	0.49
1:B:251:ILE:HG21	1:D:384:MET:HE1	1.94	0.49
1:C:190:LYS:HE2	6:C:1141:HOH:O	2.13	0.49
1:A:50:ASN:HD21	1:A:139:ILE:HA	1.77	0.48
1:A:316:VAL:HG12	1:A:322:LYS:HA	1.96	0.48
1:C:242:GLU:HB2	1:C:245:THR:HG23	1.96	0.48
1:B:50:ASN:HD21	1:B:139:ILE:HA	1.78	0.48
1:C:372:MET:HE3	1:C:404:PRO:HG3	1.96	0.48
1:B:95:ILE:HD11	1:B:101:ARG:HB2	1.96	0.47
1:C:50:ASN:HD21	1:C:139:ILE:HA	1.80	0.47
1:C:95:ILE:HD11	1:C:101:ARG:HB2	1.97	0.47
1:D:109:MET:HE3	1:D:113:GLY:HA2	1.97	0.47
1:A:256:ASP:HB3	1:A:502:VAL:HG21	1.95	0.46
1:B:268:LEU:HD12	1:D:318:ALA:HB1	1.97	0.46
1:A:416:ARG:HE	5:A:606:GOL:C2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:ALA:HB1	1:D:357:VAL:HG12	1.97	0.46
1:C:40:ASN:HD22	1:C:40:ASN:N	2.12	0.45
1:D:370:HIS:CE1	1:D:408:PRO:HG2	2.52	0.44
1:D:294:GLN:HE21	1:D:294:GLN:HA	1.83	0.44
1:D:316:VAL:HG12	1:D:322:LYS:HA	1.98	0.44
1:D:69:ALA:HB1	5:D:602:GOL:H31	2.00	0.43
1:A:372:MET:HE2	1:A:375:TYR:HB2	2.00	0.43
1:A:384:MET:HE2	1:A:384:MET:C	2.44	0.43
1:C:266:ILE:HG23	1:C:270:ASN:ND2	2.34	0.43
1:C:316:VAL:HG12	1:C:322:LYS:HA	2.00	0.43
1:A:503:HIS:HD2	1:D:405:GLY:O	2.02	0.43
1:D:256:ASP:HB3	1:D:502:VAL:HG21	2.01	0.43
1:B:256:ASP:HB3	1:B:502:VAL:HG21	2.01	0.42
1:B:372:MET:HE3	1:B:404:PRO:HG3	2.01	0.42
1:C:384:MET:C	1:C:384:MET:HE2	2.45	0.42
1:D:136:ILE:HD11	1:D:143:LYS:N	2.32	0.42
1:A:173:THR:HG22	6:A:920:HOH:O	2.19	0.42
1:D:40:ASN:HD22	1:D:40:ASN:N	2.13	0.41
1:A:429:ALA:HA	1:A:430:THR:HA	1.87	0.41
1:B:440:GLN:NE2	6:B:709:HOH:O	2.53	0.41
1:A:294:GLN:HE21	1:A:294:GLN:HA	1.86	0.41
1:C:245:THR:HG21	6:C:992:HOH:O	2.21	0.41
1:A:109:MET:HE2	1:C:166:THR:HG21	2.02	0.41
1:B:294:GLN:HE21	1:B:294:GLN:HA	1.86	0.41
1:D:136:ILE:HA	1:D:136:ILE:HD12	1.77	0.41
1:D:372:MET:HE3	1:D:404:PRO:HG3	2.03	0.41
1:B:246:ARG:HG2	1:B:258:ILE:HB	2.03	0.41
1:B:429:ALA:HA	1:B:430:THR:HA	1.86	0.41
1:C:105:ARG:HD3	6:C:842:HOH:O	2.20	0.41
1:D:105:ARG:HD3	6:D:1030:HOH:O	2.20	0.41
1:C:335:TYR:OH	1:C:422:GLN:NE2	2.54	0.40
1:C:372:MET:HE2	1:C:375:TYR:HB2	2.03	0.40
1:C:294:GLN:HA	1:C:294:GLN:HE21	1.86	0.40
1:D:335:TYR:OH	1:D:422:GLN:NE2	2.55	0.40
1:D:384:MET:HE2	1:D:384:MET:C	2.47	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	494/499 (99%)	477 (97%)	17 (3%)	0	100	100
1	B	493/499 (99%)	475 (96%)	18 (4%)	0	100	100
1	C	495/499 (99%)	478 (97%)	17 (3%)	0	100	100
1	D	490/499 (98%)	473 (96%)	17 (4%)	0	100	100
All	All	1972/1996 (99%)	1903 (96%)	69 (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	424/428 (99%)	414 (98%)	10 (2%)	43	20
1	B	423/428 (99%)	413 (98%)	10 (2%)	43	20
1	C	425/428 (99%)	418 (98%)	7 (2%)	55	34
1	D	421/428 (98%)	411 (98%)	10 (2%)	43	20
All	All	1693/1712 (99%)	1656 (98%)	37 (2%)	45	23

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	98	LYS

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Mol	Chain	Res	Type
1	A	136	ILE
1	A	260	THR
1	A	267	GLN
1	A	299	ASP
1	A	357	VAL
1	A	384	MET
1	A	463	LEU
1	A	505	LYS
1	B	33	ARG
1	B	40	ASN
1	B	98	LYS
1	B	105	ARG
1	B	136	ILE
1	B	260	THR
1	B	299	ASP
1	B	319	LEU
1	B	463	LEU
1	B	467	LYS
1	C	40	ASN
1	C	245	THR
1	C	260	THR
1	C	299	ASP
1	C	357	VAL
1	C	384	MET
1	C	398	VAL
1	D	31	GLU
1	D	40	ASN
1	D	136	ILE
1	D	138	LYS
1	D	260	THR
1	D	267	GLN
1	D	299	ASP
1	D	357	VAL
1	D	384	MET
1	D	463	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	50	ASN
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	62	GLN
1	A	294	GLN
1	A	370	HIS
1	A	396	ASN
1	A	411	ASN
1	A	420	ASN
1	A	422	GLN
1	A	440	GLN
1	A	503	HIS
1	B	40	ASN
1	B	50	ASN
1	B	54	ASN
1	B	62	GLN
1	B	294	GLN
1	B	370	HIS
1	B	396	ASN
1	B	411	ASN
1	B	412	GLN
1	B	420	ASN
1	B	422	GLN
1	B	440	GLN
1	B	516	ASN
1	C	40	ASN
1	C	50	ASN
1	C	54	ASN
1	C	62	GLN
1	C	286	HIS
1	C	294	GLN
1	C	396	ASN
1	C	412	GLN
1	C	420	ASN
1	C	422	GLN
1	C	503	HIS
1	C	516	ASN
1	D	40	ASN
1	D	50	ASN
1	D	54	ASN
1	D	62	GLN
1	D	294	GLN
1	D	370	HIS
1	D	396	ASN
1	D	411	ASN

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Mol	Chain	Res	Type
1	D	420	ASN
1	D	422	GLN
1	D	440	GLN

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 ⓘ

17 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	B	603	-	3,3,3	0.35	0	2,2,2	0.49	0
3	EDO	C	602	-	3,3,3	0.57	0	2,2,2	0.32	0
2	SO4	C	601	-	4,4,4	0.41	0	6,6,6	0.19	0
3	EDO	A	604	-	3,3,3	0.42	0	2,2,2	0.51	0
3	EDO	C	603	-	3,3,3	0.35	0	2,2,2	0.73	0
2	SO4	D	601	-	4,4,4	0.39	0	6,6,6	0.10	0
5	GOL	A	606	-	5,5,5	0.05	0	5,5,5	0.72	0
5	GOL	D	602	-	5,5,5	0.08	0	5,5,5	0.13	0
3	EDO	B	602	-	3,3,3	0.48	0	2,2,2	0.37	0
2	SO4	A	602	-	4,4,4	0.13	0	6,6,6	0.33	0
2	SO4	B	601	-	4,4,4	0.31	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	607	-	3,3,3	0.68	0	2,2,2	0.18	0
2	SO4	A	603	-	4,4,4	0.29	0	6,6,6	0.21	0
2	SO4	A	601	-	4,4,4	0.34	0	6,6,6	0.39	0
3	EDO	B	604	-	3,3,3	0.42	0	2,2,2	0.37	0
3	EDO	D	603	-	3,3,3	0.56	0	2,2,2	0.26	0
4	PEG	A	605	-	6,6,6	0.17	0	5,5,5	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
3	EDO	B	603	-	-	0/1/1/1	-
3	EDO	C	602	-	-	0/1/1/1	-
3	EDO	A	604	-	-	1/1/1/1	-
3	EDO	C	603	-	-	1/1/1/1	-
5	GOL	A	606	-	-	0/4/4/4	-
3	EDO	B	602	-	-	0/1/1/1	-
3	EDO	A	607	-	-	0/1/1/1	-
5	GOL	D	602	-	-	0/4/4/4	-
3	EDO	B	604	-	-	0/1/1/1	-
3	EDO	D	603	-	-	0/1/1/1	-
4	PEG	A	605	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	603	EDO	O1-C1-C2-O2
3	A	604	EDO	O1-C1-C2-O2
4	A	605	PEG	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	606	GOL	3	0
5	D	602	GOL	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	491/499 (98%)	-0.25	4 (0%)	82 87	9, 19, 37, 65	5 (1%)
1	B	491/499 (98%)	-0.12	6 (1%)	76 81	9, 24, 46, 61	4 (0%)
1	C	491/499 (98%)	-0.24	11 (2%)	62 70	8, 20, 40, 54	6 (1%)
1	D	491/499 (98%)	-0.14	7 (1%)	73 79	13, 22, 41, 57	1 (0%)
All	All	1964/1996 (98%)	-0.19	28 (1%)	73 79	8, 21, 42, 65	16 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	521	GLY	5.2
1	A	136	ILE	4.2
1	A	521	GLY	3.7
1	A	137	LYS	3.6
1	C	521	GLY	3.5
1	C	402	TYR	3.4
1	C	361	GLY	3.4
1	C	401	THR	3.3
1	D	137	LYS	3.0
1	C	406	SER	2.9
1	C	403	ALA	2.9
1	B	365	THR	2.8
1	C	404	PRO	2.7
1	D	136	ILE	2.7
1	D	521	GLY	2.7
1	C	365	THR	2.6
1	B	398	VAL	2.6
1	A	138	LYS	2.5
1	D	361	GLY	2.4
1	D	403	ALA	2.4
1	D	365	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	401	THR	2.3
1	C	405	GLY	2.3
1	C	407	PHE	2.2
1	C	400	LYS	2.2
1	D	406	SER	2.1
1	B	229	LYS	2.1
1	B	234	LYS	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	SO4	A	603	5/5	0.77	0.14	51,55,58,60	0
3	EDO	B	603	4/4	0.80	0.16	43,45,46,47	0
5	GOL	A	606	6/6	0.80	0.19	51,55,55,57	0
4	PEG	A	605	7/7	0.83	0.17	34,50,64,67	0
3	EDO	B	604	4/4	0.83	0.17	35,40,45,48	0
3	EDO	C	603	4/4	0.87	0.18	41,43,45,47	0
3	EDO	B	602	4/4	0.88	0.16	43,44,48,48	0
3	EDO	A	604	4/4	0.89	0.12	31,32,34,35	0
3	EDO	D	603	4/4	0.89	0.13	45,45,46,46	0
2	SO4	C	601	5/5	0.90	0.10	46,50,52,53	0
3	EDO	C	602	4/4	0.90	0.11	15,24,32,34	0
5	GOL	D	602	6/6	0.91	0.10	37,43,45,47	0
2	SO4	B	601	5/5	0.93	0.09	38,40,42,43	0
2	SO4	D	601	5/5	0.93	0.10	49,50,52,54	0
3	EDO	A	607	4/4	0.94	0.10	15,24,30,34	0
2	SO4	A	601	5/5	0.94	0.09	38,42,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	602	5/5	0.97	0.09	31,36,38,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.