



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 01:28 AM UTC

PDB ID : 1SZS / pdb_00001szs
Title : The structure of gamma-aminobutyrate aminotransferase mutant: I50Q
Authors : Liu, W.; Peterson, P.E.; Langston, J.A.; Jin, X.; Zhou, X.; Fisher, A.J.; Toney, M.D.
Deposited on : 2004-04-06
Resolution : 2.10 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

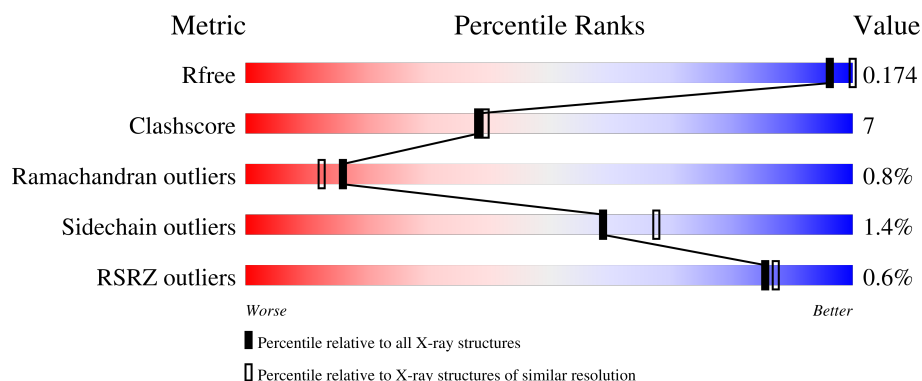
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

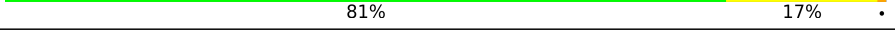
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	426	
1	B	426	
1	C	426	
1	D	426	

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
3	EDO	A	1232	-	-	X	-
3	EDO	B	1229	-	-	X	-
3	EDO	C	1230	-	-	X	-
3	EDO	D	1231	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14301 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.

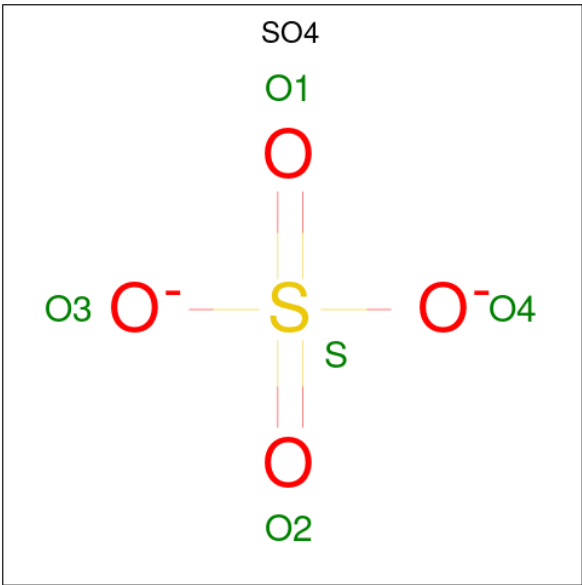
- Molecule 1 is a protein called 4-aminobutyrate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	3	0
			3228	2037	566	607	18			
1	B	425	Total	C	N	O	S	1	3	0
			3228	2037	566	607	18			
1	C	425	Total	C	N	O	S	0	3	0
			3228	2037	566	607	18			
1	D	425	Total	C	N	O	S	0	3	0
			3228	2037	566	607	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	GLN	ILE	engineered mutation	UNP P22256
B	50	GLN	ILE	engineered mutation	UNP P22256
C	50	GLN	ILE	engineered mutation	UNP P22256
D	50	GLN	ILE	engineered mutation	UNP P22256

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



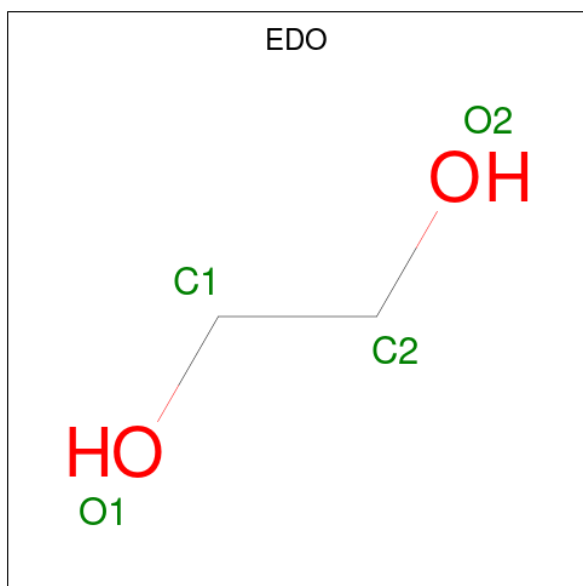
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

Continued on next page...

Continued from previous page...

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

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



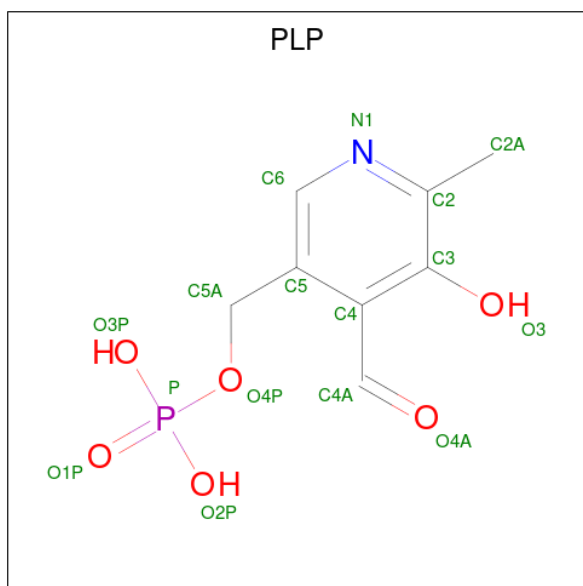
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total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

Continued on next page...

Continued from previous page...

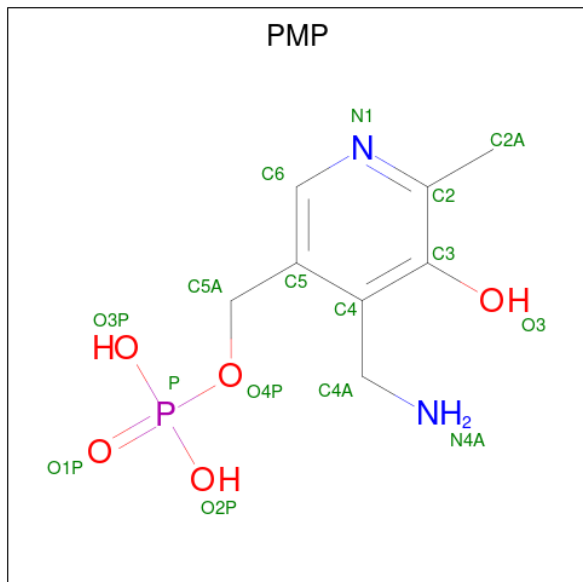
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
4	C	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
4	D	1	Total	C	N	O	P	0	1
			15	8	1	5	1		

- Molecule 5 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: $C_8H_{13}N_2O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			16	8	2	5	1		
5	B	1	Total	C	N	O	P	0	1
			16	8	2	5	1		
5	C	1	Total	C	N	O	P	0	1
			16	8	2	5	1		
5	D	1	Total	C	N	O	P	0	1
			16	8	2	5	1		

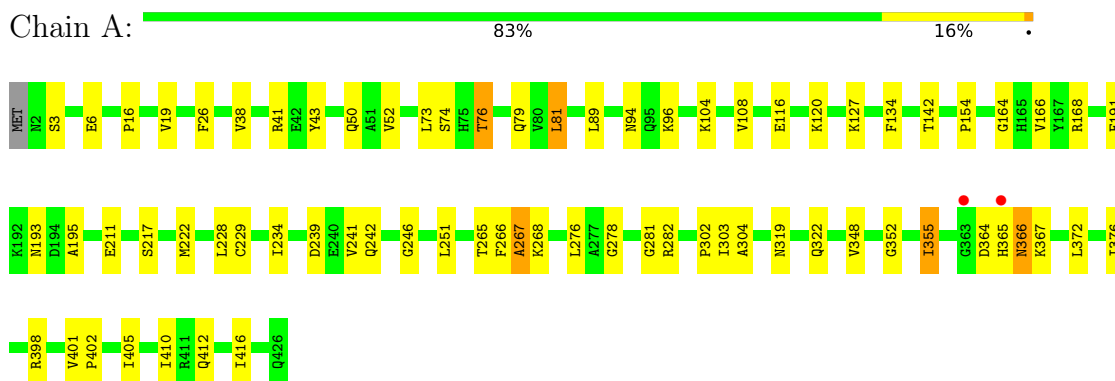
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	280	Total	O	0	0
			280	280		
6	B	298	Total	O	0	0
			298	298		
6	C	255	Total	O	0	0
			255	255		
6	D	289	Total	O	0	0
			289	289		

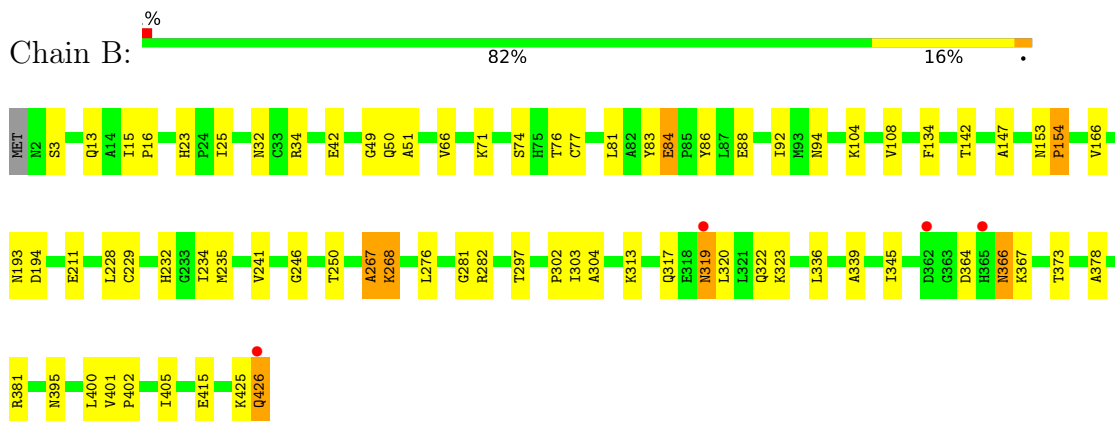
3 Residue-property plots

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.

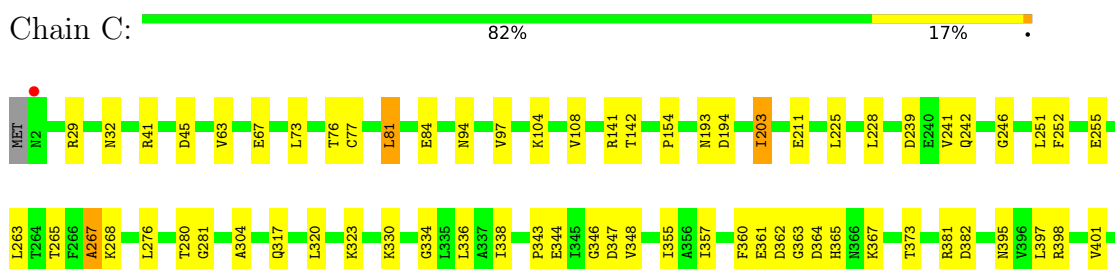
• Molecule 1: 4-aminobutyrate aminotransferase



• Molecule 1: 4-aminobutyrate aminotransferase

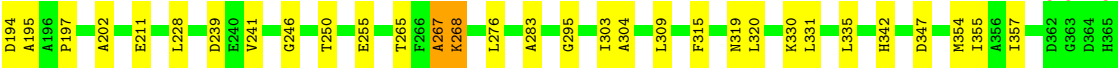
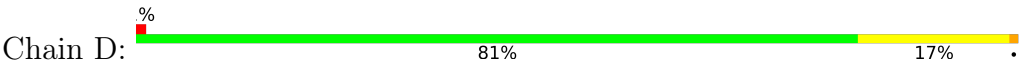


• Molecule 1: 4-aminobutyrate aminotransferase





● Molecule 1: 4-aminobutyrate aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.10Å 108.10Å 301.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.10) 95.8 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.169 , 0.206 0.173 , 0.174	Depositor DCC
R_{free} test set	5783 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14301	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: EDO, PLP, SO4, PMP

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	0.65	0/3287	1.00	10/4447 (0.2%)
1	B	0.65	0/3287	1.00	11/4447 (0.2%)
1	C	0.62	0/3287	0.98	9/4447 (0.2%)
1	D	0.66	0/3287	1.00	14/4447 (0.3%)
All	All	0.64	0/13148	0.99	44/17788 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	246	GLY	N-CA-C	7.34	124.75	115.21
1	C	246	GLY	N-CA-C	6.94	124.59	115.36
1	A	246	GLY	N-CA-C	6.89	124.53	115.36
1	B	246	GLY	N-CA-C	6.61	124.15	115.36
1	B	194	ASP	N-CA-C	6.54	122.14	114.04
1	D	283	ALA	N-CA-C	6.50	118.92	111.11
1	D	193	ASN	N-CA-C	6.39	121.33	112.45
1	B	166	VAL	N-CA-C	-6.34	98.38	107.77
1	D	76	THR	N-CA-C	-6.03	107.15	114.75
1	A	410	ILE	N-CA-C	-6.01	104.88	110.53
1	B	147	ALA	N-CA-C	-5.99	104.83	111.36
1	D	166	VAL	N-CA-C	-5.98	99.01	107.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	VAL	N-CA-C	-5.97	99.03	107.75
1	B	193	ASN	N-CA-C	5.85	120.55	113.41
1	A	142	THR	N-CA-C	-5.69	102.10	110.52
1	D	194	ASP	N-CA-C	5.68	120.73	113.18
1	C	193	ASN	N-CA-C	5.64	120.29	112.90
1	D	168	ARG	N-CA-C	5.64	117.72	108.52
1	A	134	PHE	N-CA-C	5.61	119.12	110.42
1	B	142	THR	N-CA-C	-5.58	102.26	110.52
1	A	168	ARG	N-CA-C	5.54	117.55	108.52
1	B	134	PHE	N-CA-C	5.53	118.71	110.14
1	A	193	ASN	N-CA-C	5.51	120.11	112.45
1	D	84	GLU	N-CA-C	5.48	120.94	113.16
1	C	142	THR	N-CA-C	-5.43	102.71	110.59
1	B	3	SER	N-CA-C	-5.39	100.87	109.23
1	C	45	ASP	N-CA-C	5.39	117.48	107.99
1	C	203	ILE	N-CA-C	-5.37	99.91	107.75
1	D	202	ALA	N-CA-C	5.33	116.94	108.79
1	A	355	ILE	N-CA-C	5.33	116.96	108.87
1	B	232	HIS	N-CA-C	5.31	119.73	112.88
1	A	76	THR	N-CA-C	-5.26	108.12	114.75
1	D	354	MET	N-CA-C	-5.25	102.30	109.71
1	B	250	THR	N-CA-C	-5.21	101.45	109.52
1	C	355	ILE	N-CA-C	5.19	116.44	108.71
1	C	141	ARG	N-CA-C	5.13	118.85	112.59
1	A	348	VAL	N-CA-C	-5.09	100.24	107.77
1	D	355	ILE	N-CA-C	5.09	116.29	108.71
1	C	317	GLN	N-CA-C	5.05	116.78	111.28
1	C	194	ASP	N-CA-C	5.05	121.55	110.80
1	D	250	THR	N-CA-C	-5.04	101.72	109.52
1	B	84	GLU	N-CA-C	5.03	120.31	113.16
1	D	342	HIS	CA-C-N	5.02	125.30	119.47
1	D	342	HIS	C-N-CA	5.02	125.30	119.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	393	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3228	0	3235	40	0
1	B	3228	0	3235	50	0
1	C	3228	0	3236	47	0
1	D	3228	0	3235	45	0
2	A	20	0	0	1	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	25	0	0	1	0
3	A	20	0	25	6	0
3	B	16	0	20	7	0
3	C	12	0	15	8	0
3	D	20	0	25	8	0
4	A	15	0	7	0	0
4	B	15	0	7	0	0
4	C	15	0	7	0	0
4	D	15	0	7	0	0
5	A	16	0	10	1	0
5	B	16	0	10	1	0
5	C	16	0	10	0	0
5	D	16	0	10	3	0
6	A	280	0	0	4	0
6	B	298	0	0	5	0
6	C	255	0	0	6	0
6	D	289	0	0	6	0
All	All	14301	0	13094	182	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 7.

All (182) 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:D:25:ILE:HD11	1:D:381:ARG:HD3	1.51	0.93
1:B:25:ILE:HD11	1:B:381:ARG:HD3	1.62	0.81
3:C:1224:EDO:H22	1:D:81:LEU:HD12	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:ARG:HH22	3:C:1230:EDO:H22	1.47	0.77
1:D:398:ARG:HH22	3:D:1231:EDO:H12	1.50	0.76
1:D:268[B]:LYS:HE3	5:D:1274[B]:PMP:H4A2	1.68	0.75
1:B:401:VAL:HG21	1:B:405:ILE:HD12	1.71	0.72
3:B:1229:EDO:O1	6:B:1568:HOH:O	2.08	0.71
1:C:357:ILE:HD11	1:C:397:LEU:HD12	1.73	0.70
1:B:13:GLN:HG3	6:B:1386:HOH:O	1.92	0.69
1:A:268[B]:LYS:HE2	5:A:1271[B]:PMP:H4A2	1.73	0.69
3:C:1230:EDO:O1	6:C:1527:HOH:O	2.12	0.67
1:B:319:ASN:ND2	6:B:1313:HOH:O	2.27	0.67
1:B:211:GLU:OE2	3:B:1229:EDO:H21	1.95	0.66
1:D:241:VAL:HG13	1:D:267:ALA:HB3	1.77	0.64
1:C:239:ASP:HA	1:C:265:THR:OG1	1.98	0.64
1:D:409:GLN:HG2	6:D:1551:HOH:O	1.98	0.64
1:B:211:GLU:HB2	3:B:1229:EDO:C2	2.28	0.63
1:B:50:GLN:NE2	6:B:1570:HOH:O	2.32	0.62
3:B:1229:EDO:H22	6:B:1570:HOH:O	2.00	0.61
1:C:211:GLU:OE1	3:C:1230:EDO:H21	2.00	0.61
1:D:331:LEU:O	1:D:335:LEU:HG	2.00	0.60
3:C:1230:EDO:H11	6:D:1559:HOH:O	2.00	0.60
1:C:343:PRO:HA	6:C:1419:HOH:O	2.02	0.60
1:B:84:GLU:O	1:B:88:GLU:HG3	2.02	0.60
1:B:319:ASN:ND2	1:B:322:GLN:HB3	2.17	0.60
1:D:255:GLU:OE1	6:D:1511:HOH:O	2.17	0.59
1:C:94:ASN:HD21	1:C:104:LYS:C	2.12	0.58
1:D:49:GLY:HA2	3:D:1220:EDO:H12	1.86	0.58
1:A:50:GLN:NE2	6:A:1551:HOH:O	2.37	0.57
1:A:401:VAL:HG21	1:A:405:ILE:HD12	1.87	0.57
1:A:239:ASP:HA	1:A:265:THR:OG1	2.05	0.56
1:C:211:GLU:HB2	3:C:1230:EDO:H21	1.88	0.56
1:B:364:ASP:OD2	1:B:367:LYS:HG3	2.05	0.55
1:A:94:ASN:HD21	1:A:104:LYS:C	2.14	0.55
1:C:81:LEU:HD23	1:D:27:ALA:HB2	1.87	0.55
1:C:362:ASP:C	1:C:364:ASP:H	2.15	0.55
1:D:73:LEU:C	1:D:73:LEU:HD12	2.32	0.54
1:A:211:GLU:HB2	3:A:1232:EDO:C1	2.36	0.54
1:C:84:GLU:OE1	6:C:1486:HOH:O	2.18	0.54
1:D:228:LEU:C	1:D:228:LEU:HD23	2.33	0.54
1:D:398:ARG:NH2	3:D:1231:EDO:H12	2.23	0.53
1:C:361:GLU:HB3	1:C:367:LYS:HB3	1.90	0.53
1:B:313:LYS:O	1:B:317:GLN:HG3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLN:NE2	2:A:1213:SO4:O2	2.40	0.53
1:C:362:ASP:O	1:C:364:ASP:N	2.42	0.53
1:A:276:LEU:HB2	1:A:304:ALA:HB1	1.91	0.52
1:B:74:SER:O	1:B:302:PRO:HD2	2.09	0.52
1:B:378:ALA:HA	3:B:1217:EDO:H22	1.91	0.52
1:D:50:GLN:NE2	6:D:1560:HOH:O	2.41	0.52
1:C:398:ARG:NH2	3:C:1230:EDO:H22	2.22	0.52
1:D:268[B]:LYS:NZ	5:D:1274[B]:PMP:N4A	2.57	0.52
1:D:211:GLU:HB2	3:D:1231:EDO:C1	2.40	0.52
1:D:319:ASN:ND2	6:D:1281:HOH:O	2.42	0.52
1:A:319:ASN:ND2	1:A:322:GLN:HB3	2.24	0.52
1:D:191:PHE:HA	1:D:195:ALA:O	2.08	0.52
1:B:66:VAL:HG13	1:B:303:ILE:HG23	1.92	0.52
1:C:73:LEU:HD12	1:C:73:LEU:C	2.34	0.51
1:A:76:THR:O	1:B:49:GLY:HA2	2.11	0.51
1:C:330:LYS:NZ	1:C:407:ASP:OD1	2.43	0.51
1:B:211:GLU:HB2	3:B:1229:EDO:H21	1.92	0.51
1:B:319:ASN:ND2	1:B:322:GLN:CB	2.75	0.50
1:B:15:ILE:HG23	1:B:16:PRO:HD2	1.93	0.50
1:A:412:GLN:O	1:A:416:ILE:HG13	2.11	0.50
1:C:76:THR:O	1:D:49:GLY:HA2	2.12	0.50
1:C:241:VAL:HG13	1:C:267:ALA:HB3	1.93	0.50
1:D:146:LEU:HD13	1:D:156:SER:HB3	1.93	0.49
3:A:1223:EDO:C1	1:B:81:LEU:HD12	2.41	0.49
1:C:252:PHE:O	1:C:255:GLU:HG3	2.12	0.49
1:D:211:GLU:OE2	3:D:1231:EDO:H11	2.13	0.49
1:D:268[B]:LYS:CE	5:D:1274[B]:PMP:H4A2	2.40	0.49
1:B:276:LEU:HB2	1:B:304:ALA:HB1	1.95	0.49
1:D:315:PHE:CD2	1:D:320:LEU:HB2	2.47	0.49
1:D:401:VAL:HG21	1:D:405:ILE:HD12	1.95	0.49
1:A:211:GLU:HB2	3:A:1232:EDO:O1	2.13	0.48
1:B:66:VAL:HG13	1:B:303:ILE:CG2	2.43	0.48
1:C:41:ARG:NH2	1:C:382:ASP:O	2.47	0.48
1:D:47:ALA:HB3	3:D:1220:EDO:O1	2.13	0.48
1:D:32:ASN:C	1:D:32:ASN:HD22	2.21	0.48
1:D:74:SER:HA	1:D:303:ILE:CD1	2.44	0.48
1:A:96:LYS:HB3	1:A:251:LEU:HD23	1.95	0.48
1:D:422:ASP:O	1:D:426:GLN:HG3	2.13	0.48
1:A:398:ARG:HH22	3:A:1232:EDO:H12	1.79	0.48
1:B:268[B]:LYS:HE2	5:B:1272[B]:PMP:H4A2	1.95	0.48
1:B:94:ASN:HD21	1:B:104:LYS:C	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PHE:CZ	1:A:278:GLY:HA3	2.50	0.47
1:A:81:LEU:HD12	1:B:23:HIS:HB2	1.96	0.47
1:C:336:LEU:HD23	1:C:336:LEU:HA	1.75	0.47
1:B:319:ASN:C	1:B:319:ASN:HD22	2.22	0.47
1:D:73:LEU:HD12	1:D:73:LEU:O	2.14	0.47
1:B:76:THR:O	1:B:77:CYS:HB3	2.15	0.47
1:D:94:ASN:HD21	1:D:104:LYS:C	2.22	0.47
1:C:263:LEU:HD23	1:C:281:GLY:HA3	1.97	0.47
1:C:401:VAL:HG21	1:C:405:ILE:HD12	1.96	0.47
1:C:32:ASN:C	1:C:32:ASN:HD22	2.22	0.46
1:C:425:LYS:O	1:C:426:GLN:OXT	2.33	0.46
1:A:164:GLY:HA2	6:A:1507:HOH:O	2.16	0.46
1:A:74:SER:O	1:A:302:PRO:HD2	2.16	0.46
3:A:1223:EDO:H11	1:B:81:LEU:HD12	1.98	0.46
1:D:41:ARG:NH2	1:D:382:ASP:O	2.45	0.46
1:A:229:CYS:HB3	1:A:234:ILE:O	2.16	0.46
1:B:32:ASN:HD22	1:B:32:ASN:C	2.24	0.46
1:C:228:LEU:C	1:C:228:LEU:HD23	2.41	0.46
1:C:255:GLU:HB3	6:C:1304:HOH:O	2.15	0.45
1:D:92:ILE:HD12	1:D:309:LEU:CD2	2.46	0.45
1:B:281:GLY:O	1:B:282:ARG:C	2.59	0.45
1:D:51:ALA:HB2	1:D:400:LEU:HD22	1.99	0.45
1:A:89:LEU:CD2	1:A:276:LEU:HD21	2.46	0.45
1:A:364:ASP:OD1	1:A:366:ASN:ND2	2.50	0.45
1:B:320:LEU:HD23	1:B:323:LYS:HD2	1.98	0.45
1:C:63:VAL:O	1:C:67:GLU:HG3	2.17	0.45
1:C:362:ASP:C	1:C:364:ASP:N	2.74	0.45
1:A:16:PRO:HG2	1:A:19:VAL:HG23	1.99	0.45
1:D:89:LEU:HD22	1:D:93:MET:HG2	1.99	0.45
1:D:330:LYS:NZ	1:D:407:ASP:OD1	2.50	0.45
1:D:76:THR:O	1:D:77:CYS:HB3	2.17	0.45
1:A:3:SER:OG	1:A:6:GLU:HB2	2.17	0.45
1:A:41:ARG:HD3	1:A:43:TYR:OH	2.17	0.45
1:B:83:TYR:CE1	1:B:86:TYR:HB2	2.52	0.45
1:A:127:LYS:HD3	6:A:1518:HOH:O	2.17	0.44
1:B:373:THR:OG1	1:B:395:ASN:HA	2.18	0.44
1:B:241:VAL:HG13	1:B:267:ALA:HB3	1.98	0.44
1:C:381:ARG:HD2	6:C:1367:HOH:O	2.17	0.44
1:A:74:SER:HA	1:A:303:ILE:HD13	2.00	0.44
1:A:241:VAL:HG13	1:A:267:ALA:HB3	1.99	0.44
1:A:251:LEU:HD12	1:A:251:LEU:HA	1.84	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:HG21	1:B:297:THR:CG2	2.48	0.44
1:C:320:LEU:HD23	1:C:323:LYS:HD2	2.00	0.44
1:D:239:ASP:HA	1:D:265:THR:OG1	2.18	0.43
1:D:347:ASP:O	1:D:357:ILE:HA	2.18	0.43
1:B:228:LEU:HD23	1:B:228:LEU:C	2.43	0.43
1:B:366:ASN:HD22	1:B:366:ASN:HA	1.56	0.43
1:C:346:GLY:HA3	1:C:360:PHE:HD1	1.83	0.43
1:A:242:GLN:HE22	3:A:1232:EDO:C2	2.31	0.43
1:B:319:ASN:HD21	1:B:322:GLN:HB2	1.83	0.43
1:C:203:ILE:HG21	1:C:225:LEU:HD11	2.00	0.43
1:C:334:GLY:O	1:C:338:ILE:HG13	2.19	0.43
1:B:51:ALA:HB2	1:B:400:LEU:HD13	2.01	0.43
1:A:191:PHE:HA	1:A:195:ALA:O	2.18	0.43
1:B:34:ARG:NH1	1:B:42:GLU:OE2	2.49	0.43
1:B:364:ASP:OD2	1:B:367:LYS:HE3	2.18	0.43
1:D:211:GLU:HB2	3:D:1231:EDO:C2	2.48	0.43
1:A:116:GLU:O	1:A:120:LYS:HG3	2.19	0.42
1:C:242:GLN:HA	1:C:268[B]:LYS:HD2	2.01	0.42
1:C:239:ASP:HA	1:C:265:THR:HG1	1.80	0.42
1:A:228:LEU:C	1:A:228:LEU:HD23	2.44	0.42
1:A:352:GLY:O	1:A:355:ILE:HD11	2.19	0.42
1:B:425:LYS:C	1:B:426:GLN:HE21	2.27	0.42
1:B:153:ASN:HA	1:B:154:PRO:HA	1.90	0.42
1:D:36:TRP:HA	1:D:41:ARG:O	2.19	0.42
1:A:364:ASP:OD2	1:A:367:LYS:HG3	2.20	0.42
1:B:235:MET:HA	1:B:235:MET:HE2	2.01	0.42
1:C:373:THR:OG1	1:C:395:ASN:HA	2.20	0.42
1:A:73:LEU:C	1:A:73:LEU:HD12	2.45	0.41
1:C:357:ILE:HG12	1:C:397:LEU:HB2	2.01	0.41
3:D:1231:EDO:H12	6:D:1560:HOH:O	2.19	0.41
1:B:229:CYS:HB3	1:B:234:ILE:O	2.20	0.41
6:A:1432:HOH:O	1:B:71:LYS:HE2	2.20	0.41
1:B:381:ARG:NE	3:B:1217:EDO:O2	2.46	0.41
1:C:29:ARG:NE	6:C:1456:HOH:O	2.50	0.41
1:B:336:LEU:HD23	1:B:336:LEU:HA	1.96	0.41
1:B:339:ALA:HA	1:B:345:ILE:HD12	2.01	0.41
1:C:347:ASP:O	1:C:357:ILE:HA	2.21	0.41
1:D:151:LYS:HD3	1:D:155:TYR:HE1	1.86	0.41
1:C:76:THR:O	1:C:77:CYS:HB3	2.21	0.41
1:C:97:VAL:HG21	1:C:280:THR:HB	2.02	0.41
1:C:276:LEU:HB2	1:C:304:ALA:HB1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LEU:O	1:A:376:ILE:HG12	2.20	0.41
1:B:267:ALA:O	1:B:268[B]:LYS:C	2.63	0.41
1:A:26:PHE:O	1:A:38:VAL:HG13	2.21	0.40
1:A:217[A]:SER:OG	1:A:222:MET:HE2	2.21	0.40
1:D:191:PHE:CG	1:D:197:PRO:HG3	2.56	0.40
1:C:211:GLU:HB2	3:C:1230:EDO:C2	2.50	0.40
1:D:295:GLY:HA3	2:D:1214:SO4:O4	2.21	0.40
1:C:251:LEU:HD12	1:C:251:LEU:HA	1.96	0.40
1:A:281:GLY:O	1:A:282:ARG:C	2.64	0.40
1:C:336:LEU:HD23	1:C:348:VAL:HG21	2.03	0.40
1:D:276:LEU:HB2	1:D:304:ALA:HB1	2.03	0.40
1:B:88:GLU:O	1:B:92:ILE:HG12	2.22	0.40
1:C:344:GLU:OE2	1:C:344:GLU:N	2.47	0.40
1:C:408:ALA:HA	1:C:411:ARG:NH1	2.35	0.40
1:D:83:TYR:CE1	1:D:86:TYR:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	426/426 (100%)	408 (96%)	15 (4%)	3 (1%)	18	15
1	B	426/426 (100%)	404 (95%)	18 (4%)	4 (1%)	14	10
1	C	426/426 (100%)	405 (95%)	17 (4%)	4 (1%)	14	10
1	D	426/426 (100%)	402 (94%)	20 (5%)	4 (1%)	14	10
All	All	1704/1704 (100%)	1619 (95%)	70 (4%)	15 (1%)	16	10

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	267	ALA
1	C	363	GLY
1	A	267	ALA
1	A	365	HIS
1	C	267	ALA
1	D	267	ALA
1	B	268[A]	LYS
1	B	268[B]	LYS
1	C	365	HIS
1	D	268[A]	LYS
1	D	268[B]	LYS
1	D	108	VAL
1	A	108	VAL
1	B	108	VAL
1	C	108	VAL

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	332/330 (101%)	328 (99%)	4 (1%)	63	72
1	B	332/330 (101%)	326 (98%)	6 (2%)	51	60
1	C	332/330 (101%)	329 (99%)	3 (1%)	70	78
1	D	332/330 (101%)	326 (98%)	6 (2%)	51	60
All	All	1328/1320 (101%)	1309 (99%)	19 (1%)	59	67

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LEU
1	A	154	PRO
1	A	366	ASN
1	A	402	PRO
1	B	154	PRO
1	B	319	ASN
1	B	366	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	402	PRO
1	B	415	GLU
1	B	426	GLN
1	C	81	LEU
1	C	154	PRO
1	C	415	GLU
1	D	3	SER
1	D	89	LEU
1	D	154	PRO
1	D	163	PRO
1	D	402	PRO
1	D	415	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	69	GLN
1	A	94	ASN
1	A	242	GLN
1	A	366	ASN
1	B	13	GLN
1	B	32	ASN
1	B	94	ASN
1	B	319	ASN
1	B	366	ASN
1	B	412	GLN
1	B	426	GLN
1	C	32	ASN
1	C	94	ASN
1	C	242	GLN
1	C	317	GLN
1	C	319	ASN
1	C	419	GLN
1	D	32	ASN
1	D	50	GLN
1	D	94	ASN
1	D	317	GLN
1	D	319	ASN
1	D	322	GLN
1	D	412	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 ⓘ

40 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	A	1228	-	3,3,3	1.81	1 (33%)	2,2,2	0.68	0
3	EDO	A	1232	-	3,3,3	1.84	1 (33%)	2,2,2	0.59	0
3	EDO	B	1219	-	3,3,3	1.80	1 (33%)	2,2,2	0.58	0
2	SO4	D	1214	-	4,4,4	0.36	0	6,6,6	0.17	0
3	EDO	B	1217	-	3,3,3	1.75	1 (33%)	2,2,2	0.64	0
5	PMP	C	1273[B]	-	16,16,16	3.89	6 (37%)	22,23,23	1.54	1 (4%)
2	SO4	D	1206	-	4,4,4	0.35	0	6,6,6	0.12	0
2	SO4	A	1212	-	4,4,4	0.37	0	6,6,6	0.20	0
5	PMP	B	1272[B]	-	16,16,16	3.85	5 (31%)	22,23,23	1.54	1 (4%)
2	SO4	C	1210	-	4,4,4	0.36	0	6,6,6	0.14	0
3	EDO	D	1227	-	3,3,3	1.77	1 (33%)	2,2,2	0.55	0
3	EDO	B	1229	-	3,3,3	1.65	1 (33%)	2,2,2	0.60	0
3	EDO	A	1225	-	3,3,3	1.77	1 (33%)	2,2,2	0.48	0
2	SO4	B	1208	-	4,4,4	0.33	0	6,6,6	0.15	0
3	EDO	B	1216	-	3,3,3	1.74	1 (33%)	2,2,2	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	1226	-	3,3,3	1.81	1 (33%)	2,2,2	0.51	0
2	SO4	B	1203	-	4,4,4	0.38	0	6,6,6	0.14	0
3	EDO	D	1231	-	3,3,3	1.79	1 (33%)	2,2,2	0.71	0
2	SO4	D	1205	-	4,4,4	0.38	0	6,6,6	0.21	0
3	EDO	C	1224	-	3,3,3	1.85	1 (33%)	2,2,2	0.68	0
3	EDO	C	1230	-	3,3,3	1.98	1 (33%)	2,2,2	0.87	0
2	SO4	B	1202	-	4,4,4	0.35	0	6,6,6	0.09	0
3	EDO	A	1223	-	3,3,3	1.81	1 (33%)	2,2,2	0.55	0
5	PMP	D	1274[B]	-	16,16,16	3.81	6 (37%)	22,23,23	1.53	1 (4%)
3	EDO	A	1218	-	3,3,3	1.77	1 (33%)	2,2,2	0.62	0
2	SO4	C	1215	-	4,4,4	0.31	0	6,6,6	0.21	0
2	SO4	D	1211	-	4,4,4	0.34	0	6,6,6	0.12	0
3	EDO	D	1222	-	3,3,3	1.72	1 (33%)	2,2,2	0.63	0
2	SO4	A	1213	-	4,4,4	0.32	0	6,6,6	0.20	0
4	PLP	C	1263[A]	1	15,15,16	2.48	6 (40%)	21,22,23	1.77	5 (23%)
4	PLP	A	1261[A]	1	15,15,16	2.07	5 (33%)	21,22,23	2.64	10 (47%)
2	SO4	A	1207	-	4,4,4	0.38	0	6,6,6	0.22	0
5	PMP	A	1271[B]	-	16,16,16	3.86	6 (37%)	22,23,23	1.55	2 (9%)
2	SO4	D	1209	-	4,4,4	0.38	0	6,6,6	0.07	0
3	EDO	D	1221	-	3,3,3	1.72	1 (33%)	2,2,2	0.53	0
2	SO4	A	1201	-	4,4,4	0.39	0	6,6,6	0.13	0
3	EDO	D	1220	-	3,3,3	1.75	1 (33%)	2,2,2	0.72	0
4	PLP	D	1264[A]	-	15,15,16	2.45	7 (46%)	21,22,23	1.95	5 (23%)
2	SO4	C	1204	-	4,4,4	0.44	0	6,6,6	0.14	0
4	PLP	B	1262[A]	1	15,15,16	2.16	6 (40%)	21,22,23	2.21	8 (38%)

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	A	1228	-	-	0/1/1/1	-
3	EDO	A	1232	-	-	1/1/1/1	-
3	EDO	B	1219	-	-	0/1/1/1	-
3	EDO	B	1217	-	-	0/1/1/1	-
5	PMP	C	1273[B]	-	-	2/8/8/8	0/1/1/1
5	PMP	B	1272[B]	-	-	2/8/8/8	0/1/1/1
3	EDO	D	1227	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1229	-	-	1/1/1/1	-
3	EDO	A	1225	-	-	0/1/1/1	-
3	EDO	B	1216	-	-	0/1/1/1	-
3	EDO	C	1226	-	-	0/1/1/1	-
3	EDO	D	1231	-	-	1/1/1/1	-
3	EDO	C	1224	-	-	0/1/1/1	-
3	EDO	C	1230	-	-	1/1/1/1	-
3	EDO	A	1223	-	-	0/1/1/1	-
5	PMP	D	1274[B]	-	-	2/8/8/8	0/1/1/1
3	EDO	A	1218	-	-	0/1/1/1	-
3	EDO	D	1222	-	-	0/1/1/1	-
4	PLP	C	1263[A]	1	-	0/6/6/8	0/1/1/1
4	PLP	A	1261[A]	1	-	0/6/6/8	0/1/1/1
5	PMP	A	1271[B]	-	-	2/8/8/8	0/1/1/1
3	EDO	D	1221	-	-	0/1/1/1	-
3	EDO	D	1220	-	-	0/1/1/1	-
4	PLP	D	1264[A]	-	-	1/6/6/8	0/1/1/1
4	PLP	B	1262[A]	1	-	0/6/6/8	0/1/1/1

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1271[B]	PMP	C5-C4	11.41	1.56	1.40
5	B	1272[B]	PMP	C5-C4	11.36	1.56	1.40
5	C	1273[B]	PMP	C5-C4	11.14	1.56	1.40
5	D	1274[B]	PMP	C5-C4	10.77	1.55	1.40
5	D	1274[B]	PMP	C3-C2	8.60	1.49	1.41
5	C	1273[B]	PMP	C3-C2	8.43	1.49	1.41
5	B	1272[B]	PMP	C3-C2	8.25	1.49	1.41
5	A	1271[B]	PMP	C3-C2	8.24	1.49	1.41
4	D	1264[A]	PLP	C3-C2	4.90	1.46	1.41
5	C	1273[B]	PMP	C6-N1	4.55	1.43	1.34
4	A	1261[A]	PLP	C2-N1	4.44	1.41	1.33
4	C	1263[A]	PLP	P-O1P	4.39	1.64	1.50
5	D	1274[B]	PMP	C6-N1	4.34	1.43	1.34
5	B	1272[B]	PMP	C6-N1	4.19	1.43	1.34
4	D	1264[A]	PLP	C6-C5	4.15	1.45	1.37
5	A	1271[B]	PMP	C6-N1	4.03	1.42	1.34
4	C	1263[A]	PLP	C3-C2	3.91	1.45	1.41
4	C	1263[A]	PLP	P-O4P	-3.76	1.48	1.60
4	C	1263[A]	PLP	C6-C5	3.71	1.45	1.37
4	B	1262[A]	PLP	C3-C2	3.67	1.44	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1262[A]	PLP	C6-C5	3.56	1.44	1.37
3	C	1230	EDO	O1-C1	-3.41	1.24	1.42
4	B	1262[A]	PLP	C2-N1	3.30	1.39	1.33
4	B	1262[A]	PLP	P-O4P	-3.19	1.50	1.60
4	D	1264[A]	PLP	P-O4P	-3.18	1.50	1.60
4	A	1261[A]	PLP	P-O4P	-3.18	1.50	1.60
4	D	1264[A]	PLP	C2-N1	3.15	1.39	1.33
3	C	1224	EDO	O1-C1	-3.12	1.26	1.42
4	B	1262[A]	PLP	P-O1P	3.11	1.60	1.50
4	C	1263[A]	PLP	C2-N1	3.10	1.39	1.33
4	C	1263[A]	PLP	C6-N1	3.09	1.40	1.34
3	A	1232	EDO	O1-C1	-3.07	1.26	1.42
3	A	1223	EDO	O1-C1	-3.03	1.26	1.42
3	D	1231	EDO	O1-C1	-3.02	1.26	1.42
3	A	1228	EDO	O1-C1	-3.02	1.26	1.42
3	B	1219	EDO	O1-C1	-3.01	1.26	1.42
3	C	1226	EDO	O1-C1	-3.00	1.26	1.42
3	A	1218	EDO	O1-C1	-2.97	1.27	1.42
3	D	1220	EDO	O1-C1	-2.94	1.27	1.42
3	B	1217	EDO	O1-C1	-2.94	1.27	1.42
3	B	1216	EDO	O1-C1	-2.89	1.27	1.42
3	D	1222	EDO	O1-C1	-2.88	1.27	1.42
3	D	1227	EDO	O1-C1	-2.86	1.27	1.42
4	A	1261[A]	PLP	P-O2P	2.85	1.65	1.54
3	A	1225	EDO	O1-C1	-2.82	1.27	1.42
3	D	1221	EDO	O1-C1	-2.80	1.27	1.42
3	B	1229	EDO	O1-C1	-2.76	1.28	1.42
5	A	1271[B]	PMP	C2-N1	2.76	1.38	1.33
5	C	1273[B]	PMP	C2-N1	2.64	1.38	1.33
4	D	1264[A]	PLP	C6-N1	2.64	1.39	1.34
4	D	1264[A]	PLP	P-O1P	2.62	1.58	1.50
5	B	1272[B]	PMP	C2-N1	2.59	1.38	1.33
5	D	1274[B]	PMP	C2-N1	2.58	1.38	1.33
4	A	1261[A]	PLP	C6-C5	2.44	1.42	1.37
4	B	1262[A]	PLP	C6-N1	2.22	1.38	1.34
5	C	1273[B]	PMP	C2A-C2	2.16	1.53	1.50
5	B	1272[B]	PMP	P-O3P	-2.13	1.46	1.54
5	C	1273[B]	PMP	P-O3P	-2.10	1.47	1.54
5	A	1271[B]	PMP	P-O3P	-2.06	1.47	1.54
5	A	1271[B]	PMP	C2A-C2	2.04	1.53	1.50
5	D	1274[B]	PMP	P-O3P	-2.02	1.47	1.54
4	D	1264[A]	PLP	P-O3P	2.02	1.62	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1274[B]	PMP	C2A-C2	2.01	1.53	1.50
4	A	1261[A]	PLP	P-O1P	2.01	1.56	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1261[A]	PLP	C5A-C5-C6	-5.37	110.60	119.36
5	A	1271[B]	PMP	C2A-C2-C3	4.71	126.31	120.80
5	C	1273[B]	PMP	C2A-C2-C3	4.65	126.24	120.80
4	A	1261[A]	PLP	C4A-C4-C3	-4.63	112.80	120.52
4	B	1262[A]	PLP	C5A-C5-C6	-4.61	111.85	119.36
5	D	1274[B]	PMP	C2A-C2-C3	4.47	126.02	120.80
4	A	1261[A]	PLP	C5-C6-N1	-4.42	116.63	123.83
5	B	1272[B]	PMP	C2A-C2-C3	4.36	125.91	120.80
4	D	1264[A]	PLP	C4A-C4-C3	-4.15	113.60	120.52
4	B	1262[A]	PLP	C4A-C4-C3	-3.90	114.03	120.52
4	B	1262[A]	PLP	C5-C6-N1	-3.77	117.70	123.83
4	A	1261[A]	PLP	C5A-C5-C4	3.63	129.79	122.64
4	C	1263[A]	PLP	C4A-C4-C3	-3.61	114.51	120.52
4	D	1264[A]	PLP	C5A-C5-C6	-3.55	113.58	119.36
4	A	1261[A]	PLP	C3-C4-C5	3.45	122.73	118.59
4	D	1264[A]	PLP	C4A-C4-C5	3.36	124.41	120.94
4	C	1263[A]	PLP	C5-C6-N1	-3.28	118.50	123.83
4	A	1261[A]	PLP	C6-N1-C2	3.03	124.69	119.20
4	D	1264[A]	PLP	C5-C6-N1	-3.01	118.93	123.83
4	A	1261[A]	PLP	C3-C2-N1	-3.01	117.16	120.96
4	B	1262[A]	PLP	C4A-C4-C5	2.76	123.79	120.94
4	A	1261[A]	PLP	O4P-P-O1P	2.73	113.83	106.44
4	A	1261[A]	PLP	O2P-P-O4P	2.71	113.73	106.67
4	D	1264[A]	PLP	C3-C2-N1	-2.69	117.56	120.96
4	B	1262[A]	PLP	C3-C2-N1	-2.69	117.57	120.96
4	B	1262[A]	PLP	C5A-C5-C4	2.63	127.83	122.64
4	C	1263[A]	PLP	C3-C4-C5	2.62	121.73	118.59
4	B	1262[A]	PLP	C6-N1-C2	2.54	123.80	119.20
4	C	1263[A]	PLP	C5A-C5-C6	-2.41	115.43	119.36
4	C	1263[A]	PLP	C3-C2-N1	-2.41	117.92	120.96
4	B	1262[A]	PLP	C6-C5-C4	2.37	120.04	118.10
5	A	1271[B]	PMP	C3-C2-N1	-2.11	118.30	120.96
4	A	1261[A]	PLP	C2A-C2-N1	2.01	121.42	117.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1271[B]	PMP	C5-C4-C4A-N4A
5	B	1272[B]	PMP	C3-C4-C4A-N4A
5	B	1272[B]	PMP	C5-C4-C4A-N4A
5	C	1273[B]	PMP	C3-C4-C4A-N4A
5	C	1273[B]	PMP	C5-C4-C4A-N4A
5	D	1274[B]	PMP	C3-C4-C4A-N4A
5	D	1274[B]	PMP	C5-C4-C4A-N4A
5	A	1271[B]	PMP	C3-C4-C4A-N4A
3	C	1230	EDO	O1-C1-C2-O2
3	A	1232	EDO	O1-C1-C2-O2
3	D	1231	EDO	O1-C1-C2-O2
4	D	1264[A]	PLP	C4-C5-C5A-O4P
3	B	1229	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1232	EDO	4	0
2	D	1214	SO4	1	0
3	B	1217	EDO	2	0
5	B	1272[B]	PMP	1	0
3	B	1229	EDO	5	0
3	D	1231	EDO	6	0
3	C	1224	EDO	1	0
3	C	1230	EDO	7	0
3	A	1223	EDO	2	0
5	D	1274[B]	PMP	3	0
2	A	1213	SO4	1	0
5	A	1271[B]	PMP	1	0
3	D	1220	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	425/426 (99%)	-0.71	2 (0%) 87 88	7, 21, 37, 68	3 (0%)
1	B	425/426 (99%)	-0.72	4 (0%) 81 83	6, 20, 41, 71	3 (0%)
1	C	425/426 (99%)	-0.54	1 (0%) 91 92	8, 24, 48, 72	3 (0%)
1	D	425/426 (99%)	-0.72	3 (0%) 84 86	6, 19, 38, 72	3 (0%)
All	All	1700/1704 (99%)	-0.67	10 (0%) 85 87	6, 21, 41, 72	12 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	365	HIS	2.9
1	D	363	GLY	2.7
1	B	319	ASN	2.5
1	A	365	HIS	2.4
1	D	365	HIS	2.3
1	C	2	ASN	2.2
1	B	426	GLN	2.2
1	D	362	ASP	2.2
1	A	363	GLY	2.1
1	B	362	ASP	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 ⓘ

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	C	1204	5/5	0.72	0.14	70,70,72,72	5
2	SO4	B	1203	5/5	0.73	0.18	84,85,86,86	0
3	EDO	B	1229	4/4	0.75	0.19	46,48,49,49	0
3	EDO	C	1230	4/4	0.78	0.19	49,52,54,57	0
2	SO4	A	1201	5/5	0.79	0.15	82,82,83,83	5
2	SO4	B	1202	5/5	0.80	0.16	68,68,69,69	5
2	SO4	C	1210	5/5	0.83	0.13	74,74,75,75	0
2	SO4	D	1209	5/5	0.83	0.16	62,63,64,64	5
2	SO4	D	1205	5/5	0.84	0.15	64,64,65,66	5
3	EDO	A	1232	4/4	0.86	0.16	44,44,45,47	0
3	EDO	A	1228	4/4	0.87	0.13	48,49,50,51	0
2	SO4	B	1208	5/5	0.88	0.14	44,45,48,48	5
3	EDO	B	1217	4/4	0.89	0.13	42,44,46,49	0
2	SO4	D	1211	5/5	0.90	0.12	50,50,51,51	5
2	SO4	D	1206	5/5	0.90	0.16	48,48,50,50	5
3	EDO	D	1227	4/4	0.90	0.10	31,33,34,34	0
3	EDO	D	1231	4/4	0.90	0.13	50,50,50,51	0
2	SO4	A	1207	5/5	0.92	0.09	48,49,51,51	5
2	SO4	A	1213	5/5	0.95	0.12	36,39,42,44	0
3	EDO	C	1224	4/4	0.95	0.08	27,28,33,35	0
2	SO4	A	1212	5/5	0.95	0.10	48,51,53,54	0
3	EDO	D	1221	4/4	0.95	0.13	29,31,32,33	0
3	EDO	D	1222	4/4	0.95	0.09	32,34,38,40	0
2	SO4	D	1214	5/5	0.95	0.12	56,57,58,59	0
3	EDO	B	1219	4/4	0.95	0.10	32,35,36,38	0
3	EDO	C	1226	4/4	0.96	0.07	27,34,34,35	0
2	SO4	C	1215	5/5	0.96	0.11	41,42,48,49	0
3	EDO	A	1225	4/4	0.96	0.09	22,28,32,34	0
5	PMP	A	1271[B]	16/16	0.96	0.07	23,26,27,30	16
3	EDO	D	1220	4/4	0.97	0.07	21,23,25,26	0
3	EDO	A	1218	4/4	0.97	0.05	24,24,26,26	0
3	EDO	B	1216	4/4	0.97	0.06	21,24,26,27	0
5	PMP	B	1272[B]	16/16	0.97	0.06	21,23,24,24	16
5	PMP	D	1274[B]	16/16	0.97	0.06	22,25,26,27	16
5	PMP	C	1273[B]	16/16	0.98	0.05	19,20,22,22	16
3	EDO	A	1223	4/4	0.98	0.07	24,24,28,31	0
4	PLP	A	1261[A]	15/16	0.99	0.05	7,10,16,16	14

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PLP	B	1262[A]	15/16	0.99	0.03	5,8,13,15	15
4	PLP	C	1263[A]	15/16	0.99	0.04	12,15,17,19	15
4	PLP	D	1264[A]	15/16	0.99	0.03	2,6,8,10	15

6.5 Other polymers [i](#)

There are no such residues in this entry.