



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:29 AM GMT

PDB ID : 1SFF
Title : Structure of gamma-aminobutyrate aminotransferase complex with aminooxy-acetate
Authors : Liu, W.; Peterson, P.E.; Carter, R.J.; Zhou, X.; Langston, J.A.; Fisher, A.J.; Toney, M.D.
Deposited on : 2004-02-19
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

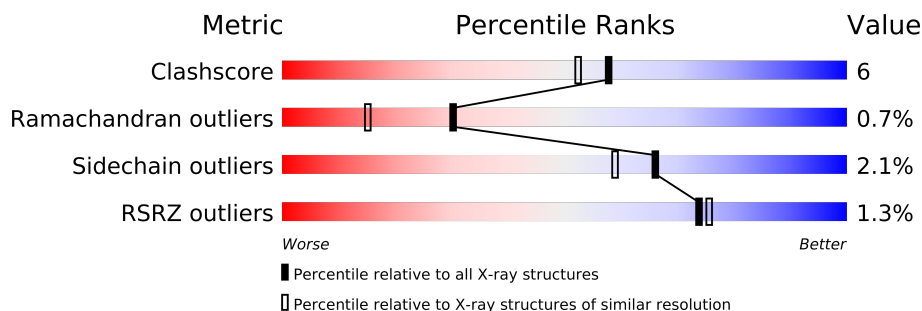
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	1307	-	X
2	SO4	B	1302	-	X
2	SO4	B	1305	-	X
2	SO4	B	1308	-	X
2	SO4	C	1303	-	X
2	SO4	C	1309	-	X
2	SO4	D	1306	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	D	1310	-	X
3	EDO	A	1401	-	X
3	EDO	A	1410	-	X
3	EDO	A	1411	-	X
3	EDO	B	1414	-	X
3	EDO	C	1409	-	X
3	EDO	D	1404	-	X
3	EDO	D	1412	-	X
3	EDO	D	1413	-	X

2 Entry composition i

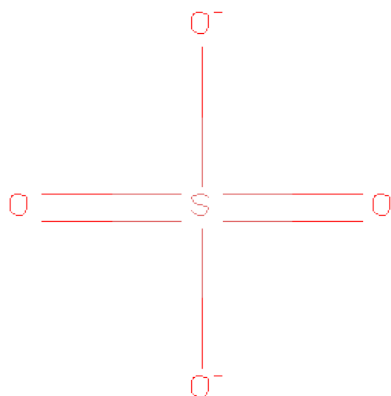
There are 5 unique types of molecules in this entry. The entry contains 14275 atoms, of which 0 are hydrogen and 0 are deuterium.

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	2	0
			3218	2032	563	605	18			
1	B	425	Total	C	N	O	S	0	2	0
			3218	2032	563	605	18			
1	C	425	Total	C	N	O	S	0	2	0
			3218	2032	563	605	18			
1	D	425	Total	C	N	O	S	0	2	0
			3218	2032	563	605	18			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



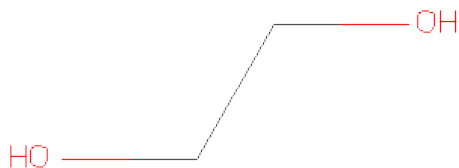
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



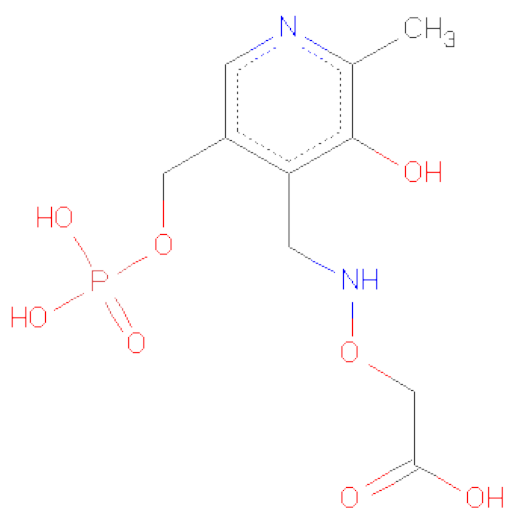
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 4 is 4'-DEOXY-4'-ACETYLYAMINO-PYRIDOXAL-5'-PHOSPHATE (three-letter code: IK2) (formula: C₁₀H₁₅N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
4	B	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
4	C	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
4	D	1	Total	C	N	O	P	0	0
			21	10	2	8	1		

- Molecule 5 is water.

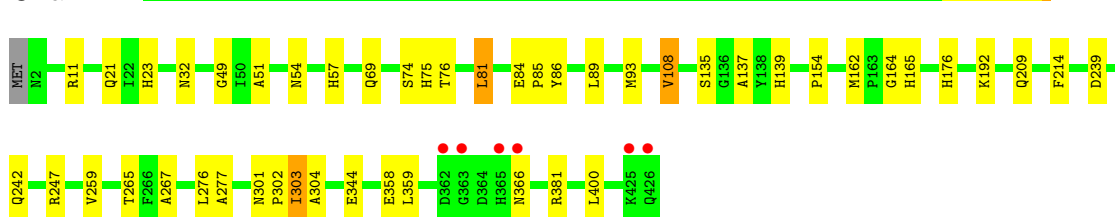
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	329	Total	O	0	0
			329	329		
5	B	316	Total	O	0	0
			316	316		
5	C	258	Total	O	0	0
			258	258		
5	D	305	Total	O	0	0
			305	305		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

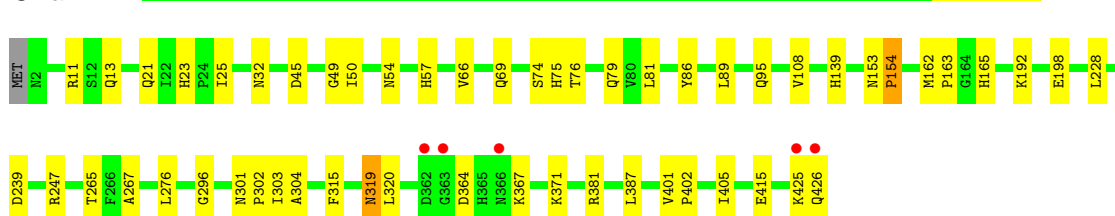
- Molecule 1: 4-aminobutyrate aminotransferase

Chain A:



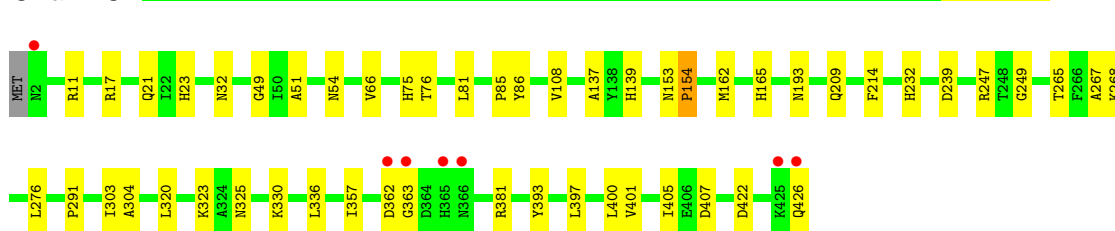
- Molecule 1: 4-aminobutyrate aminotransferase

Chain B:



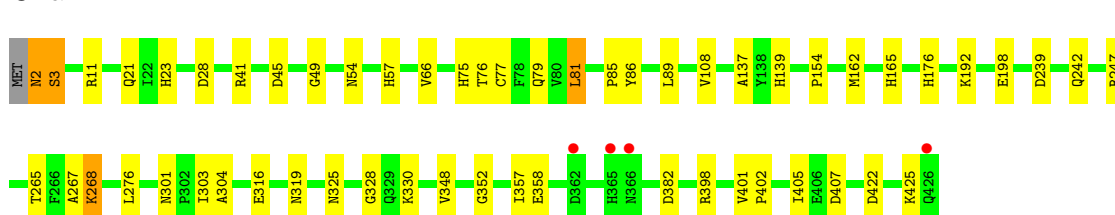
- Molecule 1: 4-aminobutyrate aminotransferase

Chain C:



- Molecule 1: 4-aminobutyrate aminotransferase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.15Å 108.15Å 301.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.90) 98.9 (29.81-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 1.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.159 , 0.186 0.168 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.6	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 160327 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14275	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IK2, SO4, EDO

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	0.72	0/3277	0.76	0/4435
1	B	0.72	0/3277	0.77	0/4435
1	C	0.65	0/3277	0.77	0/4435
1	D	0.71	0/3277	0.77	0/4435
All	All	0.70	0/13108	0.77	0/17740

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3218	0	3229	42	0
1	B	3218	0	3229	47	0
1	C	3218	0	3229	35	0
1	D	3218	0	3229	47	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	16	0	24	6	0
3	B	12	0	18	4	0
3	C	12	0	18	7	0
3	D	16	0	24	8	0
4	A	21	0	11	0	0
4	B	21	0	11	0	0
4	C	21	0	11	0	0
4	D	21	0	11	1	0
5	A	329	0	0	7	0
5	B	316	0	0	12	0
5	C	258	0	0	7	0
5	D	305	0	0	13	0
All	All	14275	0	13044	165	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (165) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:2:ASN:HD22	1:D:3:SER:H	1.15	0.94
1:C:23:HIS:HD2	1:C:381:ARG:HE	1.14	0.91
1:B:303:ILE:HG12	5:B:1672:HOH:O	1.75	0.86
1:B:198:GLU:HG3	5:B:1647:HOH:O	1.75	0.84
1:A:11:ARG:HE	1:A:21:GLN:HE21	1.27	0.83
1:D:85:PRO:HD3	3:D:1408:EDO:H22	1.60	0.82
1:D:198:GLU:HG3	5:D:1635:HOH:O	1.78	0.82
1:A:192:LYS:HE2	1:C:393:TYR:CE2	2.14	0.80
4:D:450:IK2:N4A	5:D:1718:HOH:O	2.15	0.78
1:C:11:ARG:HE	1:C:21:GLN:HE21	1.34	0.76
3:A:1401:EDO:H12	1:B:81:LEU:HD12	1.69	0.75
1:A:76:THR:HB	3:B:1402:EDO:H11	1.71	0.73
1:D:2:ASN:HD22	1:D:3:SER:N	1.86	0.72
1:A:23:HIS:HD2	1:A:381:ARG:HE	1.35	0.71
1:B:79:GLN:HE22	1:B:296:GLY:H	1.36	0.71
1:D:11:ARG:HE	1:D:21:GLN:HE21	1.36	0.71
1:C:81:LEU:HD22	3:D:1404:EDO:H21	1.73	0.70
1:B:139:HIS:HD2	1:B:239:ASP:OD2	1.75	0.70
1:B:11:ARG:HE	1:B:21:GLN:HE21	1.38	0.69
3:A:1401:EDO:H11	1:B:76:THR:HB	1.73	0.69
1:C:76:THR:HB	3:D:1404:EDO:H22	1.75	0.68
1:B:301:ASN:ND2	5:B:1672:HOH:O	2.27	0.67
1:C:232:HIS:HD2	5:C:1637:HOH:O	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:23:HIS:CD2	1:C:381:ARG:HE	2.06	0.67
1:C:85:PRO:HD3	3:C:1407:EDO:H11	1.77	0.66
1:D:75:HIS:HD2	5:D:1441:HOH:O	1.77	0.66
1:C:139:HIS:HD2	1:C:239:ASP:OD2	1.78	0.66
1:D:139:HIS:HD2	1:D:239:ASP:OD2	1.79	0.65
1:A:54:ASN:ND2	1:A:247:ARG:HH11	1.93	0.65
1:D:2:ASN:ND2	1:D:3:SER:H	1.92	0.64
1:A:75:HIS:HD2	5:A:1433:HOH:O	1.80	0.64
1:C:75:HIS:HD2	5:C:1425:HOH:O	1.79	0.63
1:B:162:MET:O	1:D:165:HIS:HE1	1.80	0.63
1:B:165:HIS:HE1	1:D:162:MET:O	1.82	0.62
3:D:1408:EDO:H21	5:D:1555:HOH:O	2.00	0.62
1:B:75:HIS:HD2	5:B:1503:HOH:O	1.83	0.61
1:A:11:ARG:HE	1:A:21:GLN:NE2	1.98	0.61
3:C:1403:EDO:H22	1:D:76:THR:HB	1.82	0.61
1:A:11:ARG:NE	1:A:21:GLN:HE21	1.96	0.61
1:B:13:GLN:HG3	5:B:1636:HOH:O	2.02	0.60
1:A:139:HIS:HD2	1:A:239:ASP:OD2	1.86	0.59
3:C:1403:EDO:H21	1:D:81:LEU:HD22	1.84	0.59
1:B:426:GLN:HG2	1:B:426:GLN:O	2.02	0.59
1:B:74:SER:O	1:B:302:PRO:HD2	2.04	0.58
1:A:57:HIS:HD2	5:B:1433:HOH:O	1.86	0.58
1:D:54:ASN:ND2	1:D:247:ARG:HH11	2.01	0.58
1:A:69:GLN:HG3	1:A:303:ILE:HD12	1.85	0.57
1:C:17:ARG:HD3	5:D:1697:HOH:O	2.04	0.57
1:B:25:ILE:HD11	1:B:381:ARG:HD3	1.86	0.57
1:B:364:ASP:OD1	1:B:367:LYS:HE3	2.04	0.57
1:B:401:VAL:HG21	1:B:405:ILE:HD12	1.87	0.57
1:A:85:PRO:HD3	3:A:1406:EDO:H11	1.86	0.57
1:A:192:LYS:CG	5:C:1586:HOH:O	2.53	0.56
1:A:165:HIS:HE1	1:C:162:MET:O	1.89	0.56
1:D:85:PRO:CD	3:D:1408:EDO:H22	2.32	0.56
1:C:54:ASN:ND2	1:C:247:ARG:HH11	2.03	0.56
1:B:11:ARG:NE	1:B:21:GLN:HE21	2.04	0.56
1:D:11:ARG:NE	1:D:21:GLN:HE21	2.03	0.55
3:A:1401:EDO:C1	1:B:81:LEU:HD12	2.36	0.55
1:C:51:ALA:HB2	1:C:400:LEU:HD22	1.89	0.55
1:D:45:ASP:OD2	3:D:1404:EDO:O2	2.22	0.54
1:B:192:LYS:HG3	5:D:1597:HOH:O	2.08	0.54
1:C:76:THR:CB	3:D:1404:EDO:H22	2.38	0.53
1:D:192:LYS:HD2	5:D:1665:HOH:O	2.09	0.53
1:C:11:ARG:NE	1:C:21:GLN:HE21	2.04	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:239:ASP:HA	1:D:265:THR:OG1	2.09	0.53
1:B:54:ASN:ND2	1:B:247:ARG:HH11	2.07	0.53
1:A:242:GLN:NE2	5:A:1740:HOH:O	2.42	0.52
1:A:139:HIS:HE1	5:A:1427:HOH:O	1.93	0.52
1:D:325:ASN:HD22	1:D:352:GLY:HA2	1.75	0.52
1:A:162:MET:O	1:C:165:HIS:HE1	1.93	0.51
3:C:1407:EDO:H22	1:D:28:ASP:HA	1.92	0.51
1:A:69:GLN:CG	1:A:303:ILE:HD12	2.39	0.51
1:D:41:ARG:NH2	1:D:382:ASP:O	2.43	0.51
1:D:66:VAL:HG13	1:D:303:ILE:HG23	1.91	0.51
5:A:1436:HOH:O	1:B:57:HIS:HD2	1.94	0.51
1:A:76:THR:CB	3:B:1402:EDO:H11	2.40	0.50
1:C:11:ARG:HE	1:C:21:GLN:NE2	2.05	0.50
1:B:11:ARG:HE	1:B:21:GLN:NE2	2.07	0.50
5:C:1421:HOH:O	1:D:57:HIS:HD2	1.94	0.50
1:B:192:LYS:CD	5:D:1597:HOH:O	2.60	0.50
1:B:139:HIS:HE1	5:B:1421:HOH:O	1.93	0.49
1:C:139:HIS:HE1	5:C:1415:HOH:O	1.95	0.49
1:C:239:ASP:HA	1:C:265:THR:OG1	2.12	0.49
1:D:401:VAL:HG21	1:D:405:ILE:HD12	1.95	0.49
1:A:137:ALA:HB1	1:A:139:HIS:CE1	2.48	0.48
1:B:228:LEU:C	1:B:228:LEU:HD23	2.34	0.48
1:C:401:VAL:HG21	1:C:405:ILE:HD12	1.94	0.48
1:D:330:LYS:NZ	1:D:407:ASP:OD1	2.47	0.48
1:B:239:ASP:HA	1:B:265:THR:OG1	2.13	0.48
1:A:276:LEU:HB2	1:A:304:ALA:HB1	1.96	0.48
1:B:66:VAL:HG13	1:B:303:ILE:CG2	2.44	0.48
1:B:79:GLN:NE2	1:B:296:GLY:H	2.07	0.48
1:B:276:LEU:HB2	1:B:304:ALA:HB1	1.94	0.48
1:D:139:HIS:HE1	5:D:1432:HOH:O	1.96	0.48
1:A:84:GLU:HG3	5:B:1470:HOH:O	2.13	0.48
1:B:371:LYS:HD3	5:B:1697:HOH:O	2.14	0.47
1:A:239:ASP:HA	1:A:265:THR:OG1	2.13	0.47
1:D:11:ARG:HE	1:D:21:GLN:NE2	2.10	0.47
1:B:319:ASN:ND2	5:B:1628:HOH:O	2.30	0.47
1:C:320:LEU:HD23	1:C:323:LYS:HD2	1.95	0.47
1:D:268:LYS:HE3	5:D:1718:HOH:O	2.15	0.47
1:D:176:HIS:HE1	1:D:358:GLU:OE1	1.98	0.47
1:A:23:HIS:CD2	1:A:381:ARG:HE	2.24	0.47
1:D:11:ARG:HH21	1:D:21:GLN:NE2	2.12	0.47
1:A:11:ARG:HH21	1:A:21:GLN:NE2	2.13	0.46
1:B:45:ASP:OD2	1:B:57:HIS:HE1	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:330:LYS:NZ	1:C:407:ASP:OD1	2.48	0.46
1:A:192:LYS:HG2	5:C:1586:HOH:O	2.15	0.46
3:C:1403:EDO:H22	1:D:76:THR:CB	2.43	0.46
1:B:153:ASN:HD22	1:B:154:PRO:HA	1.80	0.46
1:C:49:GLY:O	1:D:75:HIS:HE1	1.98	0.46
1:D:328:GLY:HA3	1:D:352:GLY:O	2.16	0.46
1:B:23:HIS:HE1	1:B:387:LEU:O	1.99	0.46
1:B:192:LYS:CG	5:D:1597:HOH:O	2.63	0.45
1:B:315:PHE:CD2	1:B:320:LEU:HB2	2.52	0.45
1:A:49:GLY:O	1:B:75:HIS:HE1	2.00	0.44
1:B:89:LEU:CD2	1:B:276:LEU:HD21	2.47	0.44
1:D:422:ASP:O	1:D:425:LYS:HG2	2.18	0.44
1:D:23:HIS:HD2	3:D:1412:EDO:O2	1.99	0.44
1:D:41:ARG:HH22	1:D:382:ASP:C	2.20	0.44
1:B:425:LYS:O	1:B:426:GLN:CD	2.56	0.44
1:D:319:ASN:ND2	5:D:1575:HOH:O	2.50	0.44
3:C:1403:EDO:H21	1:D:81:LEU:CD2	2.47	0.44
1:B:66:VAL:HG13	1:B:303:ILE:HG23	1.99	0.44
1:B:426:GLN:O	1:B:426:GLN:CG	2.65	0.44
1:A:74:SER:O	1:A:302:PRO:HD2	2.18	0.44
3:A:1401:EDO:H11	1:B:76:THR:CB	2.43	0.43
1:C:137:ALA:HB1	1:C:139:HIS:CE1	2.53	0.43
1:C:209:GLN:O	1:C:214:PHE:HA	2.18	0.43
1:B:95:GLN:NE2	5:B:1713:HOH:O	2.35	0.43
1:C:249:GLY:HA3	1:C:325:ASN:HD21	1.83	0.43
1:A:108:VAL:HG23	1:A:277:ALA:HB3	1.99	0.43
1:A:81:LEU:HD22	3:B:1402:EDO:H12	1.99	0.43
1:C:75:HIS:HE1	1:D:49:GLY:O	2.00	0.43
1:D:45:ASP:OD2	1:D:57:HIS:HE1	2.02	0.43
1:B:69:GLN:HG3	1:B:303:ILE:HD13	2.00	0.43
1:A:164:GLY:HA2	5:A:1568:HOH:O	2.18	0.43
1:C:153:ASN:HA	1:C:154:PRO:HA	1.83	0.43
1:A:81:LEU:HD22	3:B:1402:EDO:H22	2.00	0.43
1:A:89:LEU:O	1:A:93:MET:HG2	2.18	0.42
1:A:176:HIS:HE1	1:A:358:GLU:OE1	2.02	0.42
1:B:153:ASN:ND2	5:B:1614:HOH:O	2.49	0.42
1:D:268:LYS:CE	5:D:1718:HOH:O	2.66	0.42
1:A:301:ASN:HD22	1:A:304:ALA:H	1.66	0.42
1:C:357:ILE:HD11	1:C:397:LEU:HD12	2.02	0.42
1:D:301:ASN:HD22	1:D:304:ALA:H	1.66	0.42
1:D:137:ALA:HB1	1:D:139:HIS:CE1	2.54	0.42
1:A:89:LEU:CD2	1:A:276:LEU:HD21	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:192:LYS:HG3	5:C:1586:HOH:O	2.17	0.42
1:D:348:VAL:HG22	1:D:357:ILE:HG22	2.02	0.42
1:C:336:LEU:HD23	1:C:336:LEU:HA	1.84	0.41
1:A:75:HIS:HE1	1:B:49:GLY:O	2.03	0.41
3:A:1406:EDO:H12	5:A:1518:HOH:O	2.20	0.41
1:C:66:VAL:HG13	1:C:303:ILE:HG23	2.02	0.41
1:D:276:LEU:HB2	1:D:304:ALA:HB1	2.02	0.41
1:D:242:GLN:HE22	1:D:398:ARG:HH11	1.68	0.41
1:A:51:ALA:HB2	1:A:400:LEU:HD22	2.03	0.41
5:A:1568:HOH:O	3:C:1409:EDO:H21	2.19	0.41
1:A:135:SER:HA	1:C:193:ASN:OD1	2.20	0.41
1:C:422:ASP:O	1:C:426:GLN:HG3	2.21	0.41
1:A:209:GLN:O	1:A:214:PHE:HA	2.21	0.40
1:A:344:GLU:O	1:A:359:LEU:HA	2.21	0.40
1:D:77:CYS:SG	1:D:79:GLN:HG2	2.61	0.40
1:C:276:LEU:HB2	1:C:304:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	425/426 (100%)	405 (95%)	18 (4%)	2 (0%)	38	23
1	B	425/426 (100%)	407 (96%)	15 (4%)	3 (1%)	30	15
1	C	425/426 (100%)	406 (96%)	15 (4%)	4 (1%)	25	10
1	D	425/426 (100%)	406 (96%)	16 (4%)	3 (1%)	30	15
All	All	1700/1704 (100%)	1624 (96%)	64 (4%)	12 (1%)	30	15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ALA
1	B	267	ALA

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Mol	Chain	Res	Type
1	C	267	ALA
1	D	267	ALA
1	D	268	LYS
1	C	268	LYS
1	A	108	VAL
1	B	108	VAL
1	D	108	VAL
1	C	108	VAL
1	C	363	GLY
1	B	50	ILE

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	331/330 (100%)	324 (98%)	7 (2%)	66	59
1	B	331/330 (100%)	324 (98%)	7 (2%)	66	59
1	C	331/330 (100%)	326 (98%)	5 (2%)	76	73
1	D	331/330 (100%)	323 (98%)	8 (2%)	61	53
All	All	1324/1320 (100%)	1297 (98%)	27 (2%)	66	61

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	81	LEU
1	A	86	TYR
1	A	154	PRO
1	A	259	VAL
1	A	303	ILE
1	A	366	ASN
1	B	32	ASN
1	B	86	TYR
1	B	154	PRO
1	B	163	PRO
1	B	319	ASN

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Mol	Chain	Res	Type
1	B	402	PRO
1	B	415	GLU
1	C	32	ASN
1	C	86	TYR
1	C	154	PRO
1	C	291	PRO
1	C	362	ASP
1	D	2	ASN
1	D	3	SER
1	D	81	LEU
1	D	86	TYR
1	D	89	LEU
1	D	154	PRO
1	D	316	GLU
1	D	402	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	21	GLN
1	A	23	HIS
1	A	32	ASN
1	A	54	ASN
1	A	57	HIS
1	A	75	HIS
1	A	139	HIS
1	A	165	HIS
1	A	176	HIS
1	A	209	GLN
1	A	301	ASN
1	A	322	GLN
1	A	325	ASN
1	B	21	GLN
1	B	23	HIS
1	B	32	ASN
1	B	54	ASN
1	B	57	HIS
1	B	75	HIS
1	B	79	GLN
1	B	95	GLN
1	B	117	ASN

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Mol	Chain	Res	Type
1	B	139	HIS
1	B	153	ASN
1	B	165	HIS
1	B	176	HIS
1	B	188	HIS
1	B	209	GLN
1	B	242	GLN
1	B	317	GLN
1	B	319	ASN
1	B	322	GLN
1	B	325	ASN
1	B	329	GLN
1	B	366	ASN
1	C	21	GLN
1	C	23	HIS
1	C	32	ASN
1	C	54	ASN
1	C	75	HIS
1	C	117	ASN
1	C	139	HIS
1	C	165	HIS
1	C	176	HIS
1	C	209	GLN
1	C	232	HIS
1	C	242	GLN
1	C	301	ASN
1	C	317	GLN
1	C	325	ASN
1	D	2	ASN
1	D	21	GLN
1	D	23	HIS
1	D	54	ASN
1	D	57	HIS
1	D	75	HIS
1	D	117	ASN
1	D	139	HIS
1	D	165	HIS
1	D	176	HIS
1	D	209	GLN
1	D	242	GLN
1	D	301	ASN
1	D	319	ASN

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Mol	Chain	Res	Type
1	D	325	ASN
1	D	329	GLN
1	D	426	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

29 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	1301	-	4,4,4	3.39	2 (50%)	6,6,6	0.96	0
2	SO4	A	1307	-	4,4,4	3.44	2 (50%)	6,6,6	0.92	0
3	EDO	A	1401	-	3,3,3	0.60	0	2,2,2	0.20	0
3	EDO	A	1406	-	3,3,3	0.91	0	2,2,2	0.12	0
3	EDO	A	1410	-	3,3,3	0.72	0	2,2,2	0.09	0
3	EDO	A	1411	-	3,3,3	0.66	0	2,2,2	0.23	0
4	IK2	A	450	-	21,21,21	3.08	9 (42%)	29,29,29	3.63	8 (27%)
2	SO4	B	1302	-	4,4,4	3.42	2 (50%)	6,6,6	0.95	0
2	SO4	B	1305	-	4,4,4	3.42	2 (50%)	6,6,6	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	1308	-	4,4,4	3.38	2 (50%)	6,6,6	0.96	0
3	EDO	B	1402	-	3,3,3	0.65	0	2,2,2	0.22	0
3	EDO	B	1405	-	3,3,3	0.63	0	2,2,2	0.36	0
3	EDO	B	1414	-	3,3,3	0.60	0	2,2,2	0.22	0
4	IK2	B	450	-	21,21,21	3.63	9 (42%)	29,29,29	3.72	9 (31%)
2	SO4	C	1303	-	4,4,4	3.31	2 (50%)	6,6,6	0.95	0
2	SO4	C	1309	-	4,4,4	3.42	2 (50%)	6,6,6	0.95	0
2	SO4	C	1311	-	4,4,4	3.46	2 (50%)	6,6,6	0.93	0
3	EDO	C	1403	-	3,3,3	0.59	0	2,2,2	0.23	0
3	EDO	C	1407	-	3,3,3	0.82	0	2,2,2	0.18	0
3	EDO	C	1409	-	3,3,3	0.76	0	2,2,2	0.20	0
4	IK2	C	450	-	21,21,21	3.14	9 (42%)	29,29,29	3.65	7 (24%)
2	SO4	D	1304	-	4,4,4	3.38	2 (50%)	6,6,6	0.96	0
2	SO4	D	1306	-	4,4,4	3.42	2 (50%)	6,6,6	0.94	0
2	SO4	D	1310	-	4,4,4	3.42	2 (50%)	6,6,6	0.89	0
3	EDO	D	1404	-	3,3,3	0.54	0	2,2,2	0.25	0
3	EDO	D	1408	-	3,3,3	0.71	0	2,2,2	0.13	0
3	EDO	D	1412	-	3,3,3	0.74	0	2,2,2	0.18	0
3	EDO	D	1413	-	3,3,3	0.89	0	2,2,2	0.27	0
4	IK2	D	450	-	21,21,21	3.34	7 (33%)	29,29,29	3.40	7 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1301	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1307	-	-	0/0/0/0	0/0/0/0
3	EDO	A	1401	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1406	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1410	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1411	-	-	0/1/1/1	0/0/0/0
4	IK2	A	450	-	-	0/12/13/13	0/1/1/1
2	SO4	B	1302	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1305	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1308	-	-	0/0/0/0	0/0/0/0
3	EDO	B	1402	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1405	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1414	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IK2	B	450	-	-	0/12/13/13	0/1/1/1
2	SO4	C	1303	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1309	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1311	-	-	0/0/0/0	0/0/0/0
3	EDO	C	1403	-	-	0/1/1/1	0/0/0/0
3	EDO	C	1407	-	-	0/1/1/1	0/0/0/0
3	EDO	C	1409	-	-	0/1/1/1	0/0/0/0
4	IK2	C	450	-	-	0/12/13/13	0/1/1/1
2	SO4	D	1304	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1306	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1310	-	-	0/0/0/0	0/0/0/0
3	EDO	D	1404	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1408	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1412	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1413	-	-	0/1/1/1	0/0/0/0
4	IK2	D	450	-	-	0/12/13/13	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	450	IK2	C3-C2	11.45	1.49	1.40
4	D	450	IK2	C3-C2	10.07	1.48	1.40
4	C	450	IK2	C3-C2	9.56	1.47	1.40
4	D	450	IK2	OX-N4A	-7.51	1.36	1.45
4	A	450	IK2	C3-C2	7.12	1.45	1.40
4	B	450	IK2	OX-N4A	-6.73	1.37	1.45
4	A	450	IK2	OX-N4A	-6.65	1.37	1.45
4	A	450	IK2	C4A-C4	-6.11	1.44	1.51
4	C	450	IK2	C4A-C4	-5.27	1.45	1.51
4	B	450	IK2	C4A-C4	-5.21	1.45	1.51
2	D	1304	SO4	O1-S	5.17	1.63	1.47
2	B	1302	SO4	O1-S	4.99	1.63	1.47
2	A	1301	SO4	O1-S	4.98	1.63	1.47
2	D	1310	SO4	O1-S	4.97	1.63	1.47
2	C	1303	SO4	O1-S	4.96	1.63	1.47
4	C	450	IK2	OX-N4A	-4.94	1.39	1.45
2	B	1308	SO4	O1-S	4.93	1.63	1.47
2	C	1309	SO4	O1-S	4.93	1.63	1.47
2	B	1305	SO4	O1-S	4.92	1.63	1.47
2	A	1307	SO4	O1-S	4.92	1.63	1.47
2	C	1311	SO4	O3-S	-4.91	1.30	1.47
2	D	1306	SO4	O1-S	4.87	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1311	SO4	O1-S	4.79	1.62	1.47
2	A	1307	SO4	O3-S	-4.73	1.31	1.47
2	D	1306	SO4	O3-S	-4.72	1.31	1.47
4	A	450	IK2	C5-C4	4.67	1.47	1.40
2	B	1305	SO4	O3-S	-4.66	1.31	1.47
2	B	1302	SO4	O3-S	-4.66	1.31	1.47
2	D	1310	SO4	O3-S	-4.65	1.31	1.47
2	C	1309	SO4	O3-S	-4.65	1.31	1.47
2	A	1301	SO4	O3-S	-4.54	1.31	1.47
2	B	1308	SO4	O3-S	-4.51	1.31	1.47
2	C	1303	SO4	O3-S	-4.37	1.32	1.47
2	D	1304	SO4	O3-S	-4.35	1.32	1.47
4	D	450	IK2	C4A-C4	-4.33	1.46	1.51
4	B	450	IK2	C5-C4	4.31	1.46	1.40
4	C	450	IK2	C5-C4	4.21	1.46	1.40
4	B	450	IK2	C3-C4	3.79	1.46	1.40
4	D	450	IK2	C5-C4	3.59	1.45	1.40
4	C	450	IK2	C6-C5	3.35	1.45	1.37
4	D	450	IK2	C6-C5	3.31	1.45	1.37
4	B	450	IK2	C6-C5	3.28	1.45	1.37
4	D	450	IK2	O1'-C2'	3.12	1.33	1.22
4	A	450	IK2	O1'-C2'	3.04	1.33	1.22
4	D	450	IK2	C3-C4	2.94	1.45	1.40
4	B	450	IK2	O1'-C2'	2.85	1.32	1.22
4	C	450	IK2	C3-C4	2.78	1.44	1.40
4	C	450	IK2	O1'-C2'	2.70	1.31	1.22
4	C	450	IK2	C2-N1	2.69	1.38	1.33
4	A	450	IK2	C2-N1	2.63	1.38	1.33
4	A	450	IK2	C6-C5	2.37	1.43	1.37
4	A	450	IK2	C4A-N4A	-2.31	1.38	1.47
4	A	450	IK2	O3-C3	-2.30	1.31	1.37
4	B	450	IK2	C4A-N4A	-2.19	1.39	1.47
4	C	450	IK2	C2A-C2	2.18	1.54	1.50
4	B	450	IK2	C2-N1	2.04	1.37	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	450	IK2	C1'-OX-N4A	16.82	121.89	107.96
4	B	450	IK2	C1'-OX-N4A	16.69	121.79	107.96
4	A	450	IK2	C1'-OX-N4A	16.06	121.27	107.96
4	D	450	IK2	C1'-OX-N4A	15.68	120.95	107.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	450	IK2	OX-C1'-C2'	6.57	129.12	111.73
4	D	450	IK2	OX-C1'-C2'	6.51	128.94	111.73
4	C	450	IK2	OX-C1'-C2'	6.44	128.77	111.73
4	B	450	IK2	OX-C1'-C2'	6.32	128.44	111.73
4	A	450	IK2	C4-C4A-N4A	4.16	132.11	112.12
4	C	450	IK2	C4-C4A-N4A	4.06	131.62	112.12
4	B	450	IK2	C4-C4A-N4A	3.89	130.82	112.12
4	A	450	IK2	C6-C5-C4	3.87	121.04	118.10
4	B	450	IK2	C6-C5-C4	3.85	121.02	118.10
4	B	450	IK2	C4A-C4-C3	3.57	124.84	120.31
4	D	450	IK2	C4-C4A-N4A	3.51	129.00	112.12
4	C	450	IK2	C6-C5-C4	3.37	120.66	118.10
4	A	450	IK2	C4A-C4-C3	3.07	124.20	120.31
4	B	450	IK2	C5A-C5-C6	-2.92	113.76	119.28
4	A	450	IK2	C5A-C5-C6	-2.88	113.83	119.28
4	D	450	IK2	C6-C5-C4	2.62	120.09	118.10
4	A	450	IK2	OX-N4A-C4A	-2.59	103.04	106.89
4	B	450	IK2	OX-N4A-C4A	-2.57	103.07	106.89
4	C	450	IK2	C4A-C4-C3	2.51	123.50	120.31
4	A	450	IK2	C5-C6-N1	-2.51	119.33	123.86
4	C	450	IK2	C5A-C5-C6	-2.43	114.69	119.28
4	D	450	IK2	C4A-C4-C3	2.31	123.23	120.31
4	D	450	IK2	C5-C6-N1	-2.17	119.95	123.86
4	B	450	IK2	C5-C6-N1	-2.16	119.96	123.86
4	D	450	IK2	C5A-C5-C6	-2.13	115.25	119.28
4	C	450	IK2	C5-C6-N1	-2.06	120.14	123.86
4	B	450	IK2	C6-N1-C2	2.00	123.57	119.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	425/426 (99%)	-0.46	6 (1%) 72 74	7, 18, 32, 61	0
1	B	425/426 (99%)	-0.48	5 (1%) 75 78	8, 17, 34, 65	0
1	C	425/426 (99%)	-0.32	7 (1%) 68 70	9, 21, 40, 64	0
1	D	425/426 (99%)	-0.48	4 (0%) 81 83	8, 17, 34, 61	0
All	All	1700/1704 (99%)	-0.43	22 (1%) 74 75	7, 18, 36, 65	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	GLN	5.6
1	C	362	ASP	5.2
1	D	362	ASP	4.6
1	A	426	GLN	4.2
1	B	362	ASP	4.1
1	A	362	ASP	3.9
1	A	366	ASN	3.9
1	A	363	GLY	3.8
1	D	365	HIS	3.6
1	D	366	ASN	3.4
1	C	426	GLN	3.1
1	C	2	ASN	2.9
1	D	426	GLN	2.9
1	B	363	GLY	2.6
1	B	366	ASN	2.6
1	A	365	HIS	2.5
1	C	365	HIS	2.4
1	B	425	LYS	2.4
1	C	425	LYS	2.3
1	C	363	GLY	2.3
1	C	366	ASN	2.2
1	A	425	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	D	1310	5/5	0.20	16.26	60,60,64,64	5
2	SO4	D	1306	5/5	0.21	8.69	71,71,72,73	5
3	EDO	D	1413	4/4	0.15	8.43	25,25,29,30	0
2	SO4	B	1308	5/5	0.22	7.34	72,73,73,74	5
2	SO4	B	1305	5/5	0.20	6.83	78,79,79,80	0
2	SO4	C	1309	5/5	0.14	6.76	77,78,79,79	5
2	SO4	A	1307	5/5	0.17	6.66	94,94,95,95	0
3	EDO	A	1410	4/4	0.17	4.86	23,23,23,25	0
3	EDO	B	1414	4/4	0.14	4.02	31,32,41,41	0
3	EDO	A	1401	4/4	0.16	3.28	21,28,30,33	0
3	EDO	C	1409	4/4	0.16	3.12	35,41,43,45	0
2	SO4	B	1302	5/5	0.18	3.03	62,63,66,67	0
2	SO4	C	1303	5/5	0.18	2.98	61,61,65,66	0
3	EDO	D	1404	4/4	0.14	2.91	23,29,31,36	0
3	EDO	D	1412	4/4	0.12	2.59	27,33,39,40	0
3	EDO	A	1411	4/4	0.17	2.25	40,40,44,46	0
2	SO4	D	1304	5/5	0.23	1.99	64,66,68,69	0
3	EDO	B	1405	4/4	0.12	1.91	31,34,35,35	0
2	SO4	A	1301	5/5	0.15	1.61	47,48,52,54	0
3	EDO	D	1408	4/4	0.11	0.97	21,30,32,32	0
3	EDO	A	1406	4/4	0.10	0.94	19,25,29,34	0
4	IK2	C	450	21/21	0.10	0.86	12,15,41,42	0
2	SO4	C	1311	5/5	0.12	0.77	53,54,54,54	5
4	IK2	D	450	21/21	0.09	0.74	9,14,39,47	0
4	IK2	A	450	21/21	0.09	0.60	9,14,36,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	EDO	C	1403	4/4	0.11	0.49	22,26,32,34	0
4	IK2	B	450	21/21	0.08	0.30	11,15,43,45	0
3	EDO	B	1402	4/4	0.10	0.29	17,24,28,29	0
3	EDO	C	1407	4/4	0.08	0.29	19,26,26,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.