



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:19 PM GMT

PDB ID : 1SZK
Title : The structure of gamma-aminobutyrate aminotransferase mutant: E211S
Authors : Liu, W.; Peterson, P.E.; Langston, J.A.; Jin, X.; Fisher, A.J.; Toney, M.D.
Deposited on : 2004-04-05
Resolution : 2.52 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

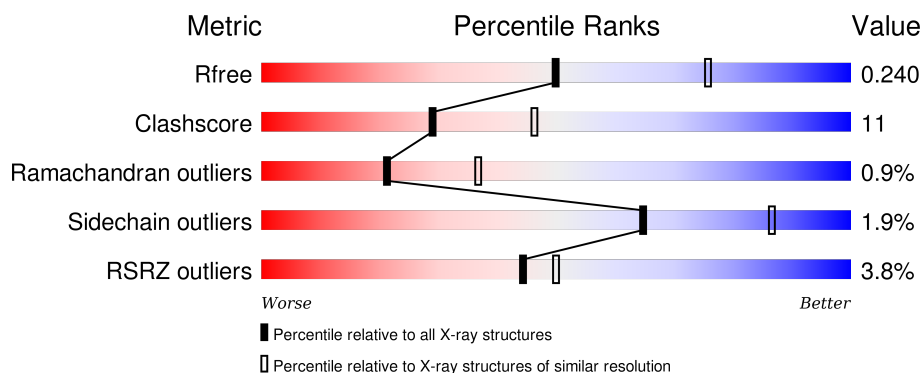
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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}	91344	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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. 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	<div> <div>3%</div> <div>79%</div> <div>19%</div> </div>
1	B	426	<div> <div>4%</div> <div>78%</div> <div>21%</div> </div>
1	C	426	<div> <div>5%</div> <div>73%</div> <div>25%</div> </div>
1	D	426	<div> <div>4%</div> <div>71%</div> <div>27%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	712	-	-	-	X
2	SO4	B	713	-	-	-	X
2	SO4	D	715	-	-	-	X
3	EDO	A	808	-	-	-	X
3	EDO	A	810	-	-	-	X
3	EDO	B	801	-	-	-	X
3	EDO	B	804	-	-	-	X
3	EDO	C	803	-	-	-	X
3	EDO	C	809	-	-	-	X
3	EDO	D	805	-	-	X	-
3	EDO	D	806	-	-	-	X
3	EDO	D	807	-	-	-	X
3	EDO	D	812	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13688 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	1	0
			3209	2027	562	602	18			
1	B	425	Total	C	N	O	S	0	0	0
			3203	2024	561	600	18			
1	C	425	Total	C	N	O	S	0	0	0
			3203	2024	561	600	18			
1	D	425	Total	C	N	O	S	0	1	0
			3209	2027	562	602	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	SER	GLU	ENGINEERED	UNP P22256
B	211	SER	GLU	ENGINEERED	UNP P22256
C	211	SER	GLU	ENGINEERED	UNP P22256
D	211	SER	GLU	ENGINEERED	UNP P22256

- 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		
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	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	D	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	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		

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

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



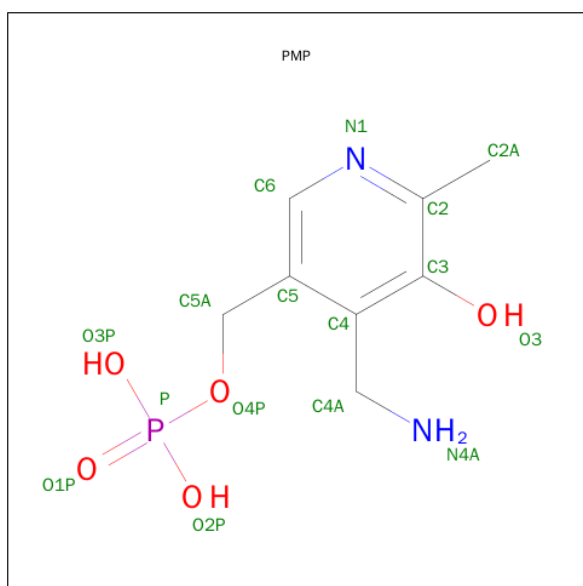
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total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

- Molecule 4 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C₈H₁₃N₂O₅P).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	179	Total	O	0	0
			179	179		
5	B	177	Total	O	0	0
			177	177		

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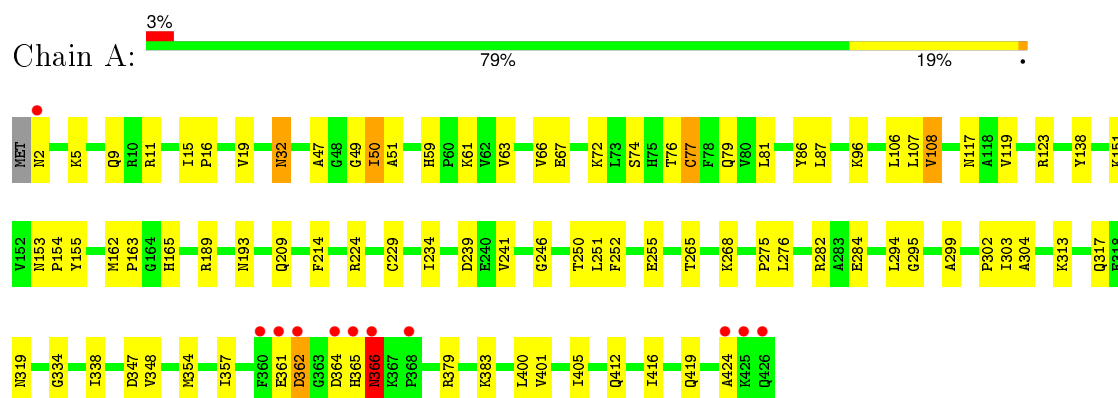
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	142	Total	O	0	0
			142	142		
5	D	175	Total	O	0	0
			175	175		

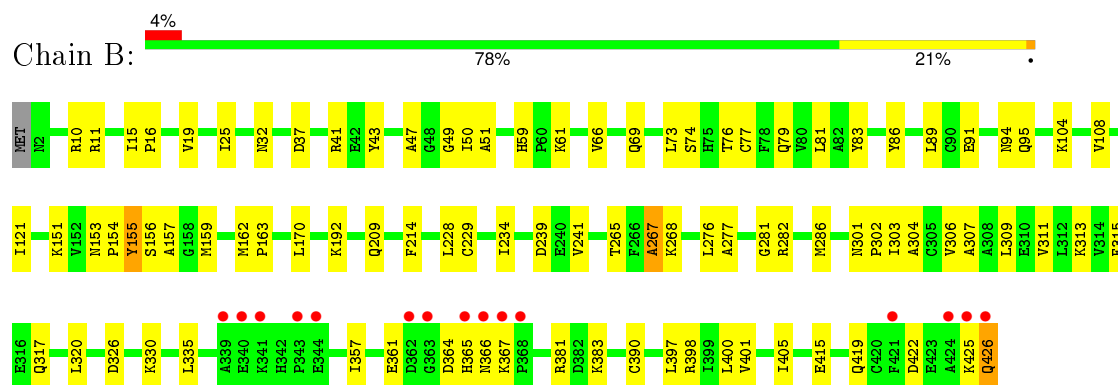
3 Residue-property plots [i](#)

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.

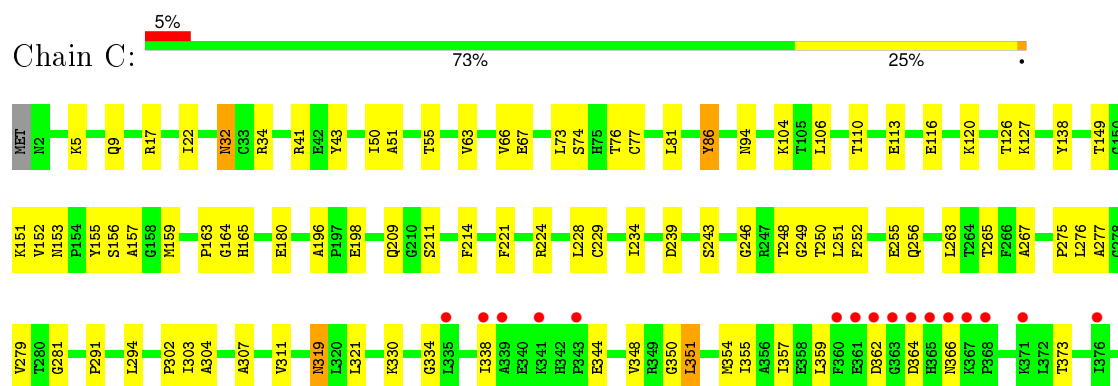
• Molecule 1: 4-aminobutyrate aminotransferase

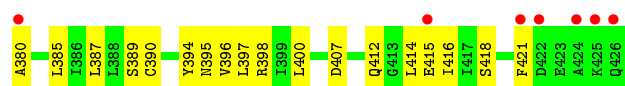


• Molecule 1: 4-aminobutyrate aminotransferase

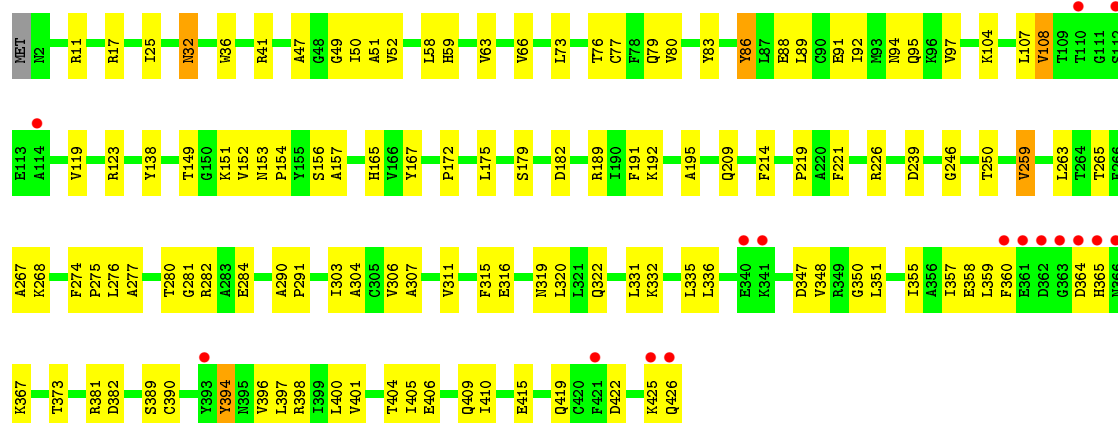


• Molecule 1: 4-aminobutyrate aminotransferase





● 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	108.26Å 108.26Å 300.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.52 47.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.52) 97.5 (47.63-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.187 , 0.240 0.187 , 0.240	Depositor DCC
R_{free} test set	3452 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.8	EDS
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 69920 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13688	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PMP, 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	0.37	0/3268	0.62	0/4423
1	B	0.38	0/3262	0.62	0/4415
1	C	0.36	0/3262	0.61	0/4415
1	D	0.38	0/3268	0.63	0/4423
All	All	0.37	0/13060	0.62	0/17676

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3209	0	3224	71	0
1	B	3203	0	3220	75	0
1	C	3203	0	3220	82	0
1	D	3209	0	3224	84	0
2	A	15	0	0	1	0
2	B	20	0	0	0	0
2	C	15	0	0	1	0
2	D	25	0	0	0	0
3	A	12	0	18	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	18	4	0
3	C	12	0	18	1	0
3	D	16	0	24	5	0
4	A	16	0	10	1	0
4	B	16	0	10	1	0
4	C	16	0	10	0	0
4	D	16	0	10	1	0
5	A	179	0	0	7	0
5	B	177	0	0	6	0
5	C	142	0	0	5	0
5	D	175	0	0	3	0
All	All	13688	0	13006	296	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 11.

All (296) 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	1.43	1.00
1:B:25:ILE:HD11	1:B:381:ARG:HD3	1.45	0.98
1:C:348:VAL:HG22	1:C:357:ILE:HG22	1.61	0.82
1:C:334:GLY:HA3	1:C:414:LEU:HD13	1.63	0.80
1:D:401:VAL:HG21	1:D:405:ILE:HD12	1.65	0.78
1:C:17:ARG:HH11	1:D:291:PRO:HD3	1.51	0.75
1:A:401:VAL:HG21	1:A:405:ILE:HD12	1.68	0.74
1:A:165:HIS:H	3:C:803:EDO:H11	1.53	0.74
1:C:350:GLY:HA3	1:C:355:ILE:HD13	1.74	0.70
1:D:364:ASP:OD2	1:D:367:LYS:HG3	1.91	0.70
5:A:857:HOH:O	1:C:157:ALA:HA	1.93	0.68
1:B:156:SER:HA	1:B:159:MET:CE	2.24	0.68
1:A:151:LYS:HD3	1:A:155:TYR:CE1	2.29	0.68
1:A:66:VAL:HG13	1:A:303:ILE:HG23	1.74	0.68
1:B:307:ALA:O	1:B:311:VAL:HG23	1.93	0.67
1:A:72:LYS:HE2	5:B:936:HOH:O	1.95	0.67
1:A:284:GLU:H	1:A:284:GLU:CD	1.99	0.66
1:B:151:LYS:HD3	1:B:155:TYR:CE1	2.31	0.65
1:B:151:LYS:HE3	1:B:153:ASN:O	1.95	0.65
1:D:88:GLU:O	1:D:92:ILE:HG13	1.97	0.65
1:C:196:ALA:HB1	1:C:198:GLU:OE2	1.98	0.63
1:C:17:ARG:NH1	1:D:291:PRO:HD3	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ASN:N	1:A:366:ASN:HD22	1.96	0.63
1:C:246:GLY:HA2	1:C:250:THR:O	1.99	0.63
1:C:76:THR:HB	3:D:805:EDO:H22	1.81	0.63
1:C:151:LYS:HE3	1:C:153:ASN:O	1.99	0.62
1:D:406:GLU:HB2	1:D:409:GLN:OE1	2.00	0.62
1:A:364:ASP:CG	1:A:366:ASN:HD21	2.03	0.61
1:B:192:LYS:HD2	5:B:951:HOH:O	2.00	0.61
1:A:63:VAL:O	1:A:67:GLU:HG3	2.01	0.60
1:C:256:GLN:OE1	1:C:351:LEU:HD21	2.01	0.60
1:D:157:ALA:HA	5:D:940:HOH:O	2.00	0.60
1:C:265:THR:HG22	1:C:279:VAL:HG22	1.83	0.59
1:B:426:GLN:N	1:B:426:GLN:NE2	2.50	0.59
1:A:276:LEU:HB2	1:A:304:ALA:HB1	1.84	0.59
1:D:358:GLU:HG2	1:D:360:PHE:CE2	2.38	0.59
1:D:41:ARG:HH22	1:D:382:ASP:C	2.05	0.59
1:C:224:ARG:HD2	5:C:879:HOH:O	2.03	0.59
1:B:315:PHE:CD2	1:B:320:LEU:HB2	2.38	0.59
1:B:303:ILE:O	1:B:306:VAL:HG22	2.03	0.59
1:C:66:VAL:HG13	1:C:303:ILE:HG23	1.86	0.58
1:D:76:THR:O	1:D:77:CYS:HB3	2.04	0.58
1:A:72:LYS:HD2	3:A:810:EDO:H12	1.85	0.58
1:C:63:VAL:O	1:C:67:GLU:HG3	2.04	0.58
1:B:157:ALA:HA	5:B:839:HOH:O	2.02	0.58
1:C:106:LEU:HD22	1:C:294:LEU:HD13	1.86	0.58
1:C:41:ARG:HG2	1:C:43:TYR:CE1	2.38	0.58
1:D:47:ALA:HB3	3:D:805:EDO:O1	2.03	0.57
1:A:76:THR:HB	3:B:801:EDO:H11	1.86	0.57
1:A:313:LYS:HB3	1:A:317:GLN:HE21	1.69	0.57
1:B:229:CYS:HB3	1:B:234:ILE:O	2.06	0.56
1:C:412:GLN:O	1:C:416:ILE:HG13	2.06	0.56
1:C:32:ASN:C	1:C:32:ASN:HD22	2.07	0.56
1:C:229:CYS:HB3	1:C:234:ILE:O	2.06	0.56
1:B:361:GLU:HB2	1:B:367:LYS:CB	2.36	0.56
1:A:209:GLN:O	1:A:214:PHE:HA	2.06	0.55
1:B:426:GLN:N	1:B:426:GLN:HE21	2.04	0.55
1:D:350:GLY:HA3	1:D:355:ILE:HD13	1.87	0.55
1:B:361:GLU:HB2	1:B:367:LYS:HB3	1.88	0.55
1:D:209:GLN:O	1:D:214:PHE:HA	2.06	0.55
1:A:5:LYS:O	1:A:9:GLN:HG3	2.07	0.55
1:A:246:GLY:HA2	1:A:250:THR:O	2.07	0.55
1:A:162:MET:HB3	1:A:163:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ILE:HG23	1:B:16:PRO:HD2	1.89	0.54
1:D:360:PHE:HB3	1:D:364:ASP:O	2.07	0.54
1:A:106:LEU:HD22	1:A:294:LEU:HD13	1.90	0.54
1:C:263:LEU:HD23	1:C:281:GLY:HA3	1.90	0.54
1:B:241:VAL:HG13	1:B:267:ALA:HB3	1.90	0.54
1:A:295:GLY:HA2	5:A:921:HOH:O	2.08	0.54
1:A:239:ASP:HA	1:A:265:THR:OG1	2.09	0.53
1:A:282:ARG:NH2	5:A:968:HOH:O	2.41	0.53
1:B:209:GLN:O	1:B:214:PHE:HA	2.09	0.53
1:A:50:ILE:HG21	2:A:712:SO4:O2	2.09	0.53
5:C:923:HOH:O	1:D:58:LEU:HD13	2.07	0.53
1:A:366:ASN:N	1:A:366:ASN:ND2	2.57	0.53
1:B:37:ASP:OD2	1:B:41:ARG:HB3	2.08	0.53
1:C:211:SER:HB3	2:C:714:SO4:O3	2.08	0.52
1:A:76:THR:O	1:A:77:CYS:HB3	2.10	0.52
1:D:415:GLU:O	1:D:419:GLN:HG3	2.08	0.52
1:D:51:ALA:HB2	1:D:400:LEU:HD22	1.92	0.52
1:C:359:LEU:HD21	1:C:421:PHE:HZ	1.75	0.52
1:D:390:CYS:SG	1:D:398:ARG:HD3	2.49	0.52
1:D:359:LEU:HD12	1:D:373:THR:HA	1.91	0.52
1:D:422:ASP:O	1:D:425:LYS:HG2	2.10	0.52
1:A:2:ASN:N	5:A:966:HOH:O	2.43	0.51
1:C:5:LYS:O	1:C:9:GLN:HG3	2.10	0.51
1:C:110:THR:OG1	1:C:113:GLU:HG3	2.11	0.51
1:B:76:THR:O	1:B:77:CYS:HB3	2.11	0.51
1:D:316:GLU:HA	1:D:316:GLU:OE1	2.10	0.50
1:B:69:GLN:HG3	1:B:303:ILE:HD13	1.93	0.50
1:D:239:ASP:HA	1:D:265:THR:OG1	2.10	0.50
1:D:389:SER:HA	1:D:396:VAL:O	2.11	0.50
1:B:66:VAL:HG13	1:B:303:ILE:HG23	1.94	0.50
1:A:383:LYS:HE3	1:A:419:GLN:HB3	1.92	0.50
1:B:426:GLN:H	1:B:426:GLN:NE2	2.09	0.50
1:A:138:TYR:HE2	4:A:750:PMP:HNA1	1.54	0.50
1:B:383:LYS:HE3	1:B:419:GLN:HB3	1.93	0.50
1:D:406:GLU:O	1:D:410:ILE:HG13	2.12	0.49
1:D:303:ILE:O	1:D:306:VAL:HG22	2.12	0.49
1:D:360:PHE:CD1	1:D:365:HIS:HA	2.47	0.49
1:C:390:CYS:SG	1:C:398:ARG:HD3	2.51	0.49
1:C:17:ARG:NH1	1:D:291:PRO:CD	2.75	0.49
1:B:214:PHE:HZ	1:B:400:LEU:HD21	1.77	0.49
1:A:108:VAL:HG12	5:A:930:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:GLU:HG2	1:C:221:PHE:HB2	1.94	0.49
1:C:55:THR:HG21	1:C:311:VAL:HG13	1.95	0.49
1:C:276:LEU:HG	1:C:277:ALA:N	2.26	0.49
1:C:380:ALA:HB1	1:C:385:LEU:HB3	1.93	0.49
1:C:138:TYR:HA	1:C:149:THR:HG23	1.94	0.49
1:C:276:LEU:HB2	1:C:304:ALA:HB1	1.94	0.49
1:A:252:PHE:O	1:A:255:GLU:HG3	2.12	0.49
1:C:66:VAL:HG13	1:C:303:ILE:CG2	2.43	0.49
1:C:17:ARG:NH1	1:D:290:ALA:HA	2.27	0.49
1:A:77:CYS:SG	1:A:79:GLN:HG2	2.53	0.49
1:D:394:TYR:CD1	1:D:394:TYR:N	2.80	0.49
1:B:74:SER:O	1:B:302:PRO:HD2	2.12	0.49
1:D:268:LYS:NZ	4:D:753:PMP:N4A	2.60	0.49
1:A:96:LYS:HB3	1:A:251:LEU:HD23	1.94	0.49
1:C:34:ARG:NH1	5:C:909:HOH:O	2.46	0.48
1:A:366:ASN:HD22	1:A:366:ASN:H	1.59	0.48
1:B:79:GLN:HG3	5:B:862:HOH:O	2.12	0.48
1:C:116:GLU:O	1:C:120:LYS:HG3	2.13	0.48
1:B:268:LYS:CE	4:B:751:PMP:H4A2	2.43	0.48
1:D:94:ASN:HD21	1:D:104:LYS:C	2.17	0.48
1:D:97:VAL:HB	1:D:280:THR:HG21	1.96	0.48
1:A:15:ILE:C	1:B:104:LYS:HD3	2.34	0.48
1:C:344:GLU:CD	1:C:344:GLU:H	2.17	0.48
1:A:412:GLN:O	1:A:416:ILE:HG13	2.12	0.48
1:C:76:THR:O	1:C:77:CYS:HB3	2.13	0.48
1:A:81:LEU:HD22	3:B:801:EDO:H12	1.96	0.47
1:D:11:ARG:HH11	1:D:11:ARG:HG2	1.79	0.47
1:A:282:ARG:HG2	1:A:284:GLU:OE1	2.14	0.47
1:B:89:LEU:HA	1:B:309:LEU:HD21	1.95	0.47
1:D:79:GLN:HG3	5:D:855:HOH:O	2.15	0.47
1:D:52:VAL:HG22	1:D:268:LYS:HA	1.96	0.47
1:D:167:TYR:HA	3:D:812:EDO:H11	1.97	0.47
1:D:36:TRP:HA	1:D:41:ARG:O	2.14	0.47
1:C:164:GLY:O	1:C:165:HIS:HB2	2.14	0.47
1:C:248:THR:HB	1:C:351:LEU:HD22	1.97	0.47
1:C:214:PHE:CZ	1:C:398:ARG:HB2	2.50	0.47
1:D:32:ASN:ND2	1:D:404:THR:OG1	2.47	0.47
1:C:126:THR:O	1:C:127:LYS:HB2	2.13	0.47
1:B:239:ASP:HA	1:B:265:THR:OG1	2.15	0.47
1:C:243:SER:HA	1:C:354:MET:CE	2.44	0.47
1:A:334:GLY:O	1:A:338:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ALA:HB2	1:C:400:LEU:HD22	1.97	0.47
1:C:152:VAL:HG13	1:C:156:SER:HB2	1.96	0.47
1:B:364:ASP:OD1	1:B:367:LYS:HE3	2.15	0.47
1:D:108:VAL:HG23	1:D:277:ALA:HB3	1.96	0.47
1:D:83:TYR:CE1	1:D:86:TYR:HB2	2.51	0.46
1:B:426:GLN:O	1:B:426:GLN:HG2	2.15	0.46
1:D:151:LYS:HE2	1:D:153:ASN:O	2.15	0.46
1:D:66:VAL:HG13	1:D:303:ILE:HG23	1.97	0.46
1:A:15:ILE:HG23	1:A:16:PRO:HD2	1.96	0.46
1:D:219:PRO:HD2	5:D:862:HOH:O	2.14	0.46
1:B:94:ASN:HD21	1:B:104:LYS:C	2.19	0.46
1:D:175:LEU:O	1:D:175:LEU:HG	2.14	0.46
1:B:83:TYR:CE1	1:B:86:TYR:HB2	2.49	0.46
1:D:263:LEU:HD23	1:D:281:GLY:HA3	1.96	0.46
1:B:156:SER:HA	1:B:159:MET:HE1	1.97	0.46
1:D:138:TYR:HA	1:D:149:THR:HG23	1.97	0.46
1:B:422:ASP:O	1:B:425:LYS:HB2	2.16	0.46
1:A:59:HIS:O	1:A:63:VAL:HG23	2.16	0.46
1:A:11:ARG:HH22	1:A:19:VAL:HG12	1.81	0.46
1:A:282:ARG:NH1	5:A:913:HOH:O	2.33	0.46
1:B:47:ALA:HB3	3:B:801:EDO:O2	2.16	0.46
1:A:49:GLY:HA2	1:B:76:THR:O	2.15	0.45
1:D:347:ASP:O	1:D:357:ILE:HA	2.16	0.45
1:A:119:VAL:O	1:A:123:ARG:HG3	2.15	0.45
1:A:364:ASP:OD2	1:A:366:ASN:ND2	2.41	0.45
1:B:108:VAL:HG23	1:B:277:ALA:HB3	1.98	0.45
1:D:59:HIS:O	1:D:63:VAL:HG23	2.16	0.45
1:A:162:MET:HB3	1:A:163:PRO:CD	2.46	0.45
1:D:91:GLU:O	1:D:95:GLN:HG2	2.16	0.45
1:A:151:LYS:HE3	1:A:153:ASN:O	2.17	0.45
1:C:155:TYR:O	1:C:159:MET:HE1	2.15	0.45
1:B:170:LEU:HD21	1:D:189:ARG:HD3	1.99	0.45
1:B:66:VAL:HG13	1:B:303:ILE:CG2	2.47	0.45
1:A:241:VAL:HG12	1:A:268:LYS:HE2	1.99	0.45
1:B:91:GLU:O	1:B:95:GLN:HG2	2.17	0.45
1:C:319:ASN:ND2	5:C:855:HOH:O	2.50	0.45
1:B:364:ASP:C	1:B:366:ASN:H	2.20	0.45
1:B:11:ARG:HG2	1:B:11:ARG:HH11	1.82	0.45
1:C:81:LEU:HD22	3:D:805:EDO:H21	1.99	0.44
1:A:107:LEU:O	1:A:299:ALA:HB1	2.17	0.44
1:D:73:LEU:HD12	1:D:73:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:SER:HA	1:A:303:ILE:CD1	2.47	0.44
1:A:108:VAL:HG11	1:A:117:ASN:ND2	2.33	0.44
1:D:284:GLU:N	1:D:284:GLU:OE2	2.39	0.44
1:B:228:LEU:HD23	1:B:228:LEU:C	2.38	0.44
1:D:172:PRO:HG3	1:D:221:PHE:CD2	2.53	0.44
1:B:51:ALA:HB2	1:B:400:LEU:HD22	2.00	0.44
1:B:276:LEU:HB2	1:B:304:ALA:HB1	1.99	0.44
1:C:373:THR:OG1	1:C:395:ASN:HA	2.18	0.44
1:B:282:ARG:HD3	5:B:950:HOH:O	2.18	0.44
1:A:106:LEU:HD13	1:B:19:VAL:CG2	2.48	0.44
1:B:301:ASN:HA	1:B:302:PRO:HD3	1.87	0.44
3:B:804:EDO:H11	1:D:165:HIS:H	1.83	0.43
1:B:121:ILE:HD13	1:B:286:MET:CE	2.48	0.43
1:C:249:GLY:O	1:C:321:LEU:HD22	2.18	0.43
1:A:229:CYS:HB3	1:A:234:ILE:O	2.19	0.43
1:A:379:ARG:NE	1:A:424:ALA:HB2	2.34	0.43
1:C:357:ILE:O	1:C:357:ILE:HG13	2.17	0.43
1:D:32:ASN:HD22	1:D:32:ASN:C	2.21	0.43
1:B:170:LEU:HD21	1:D:189:ARG:CD	2.48	0.43
1:B:151:LYS:HZ2	1:D:192:LYS:NZ	2.17	0.43
1:C:94:ASN:HD21	1:C:104:LYS:C	2.21	0.43
1:C:239:ASP:HA	1:C:265:THR:OG1	2.19	0.43
1:C:385:LEU:CD2	1:C:387:LEU:HD21	2.48	0.43
1:C:94:ASN:HA	1:C:94:ASN:HD22	1.66	0.43
1:C:338:ILE:HD13	1:C:418:SER:HA	2.00	0.43
1:D:179:SER:O	1:D:182:ASP:N	2.51	0.43
1:B:326:ASP:O	1:B:330:LYS:HG3	2.19	0.43
1:D:281:GLY:O	1:D:282:ARG:C	2.57	0.43
1:A:189:ARG:O	1:A:193:ASN:HB2	2.19	0.43
1:C:55:THR:HG23	5:C:870:HOH:O	2.18	0.43
1:A:47:ALA:HB3	3:A:808:EDO:O2	2.19	0.43
1:C:334:GLY:HA3	1:C:414:LEU:CD1	2.43	0.42
1:C:41:ARG:HG2	1:C:43:TYR:CZ	2.53	0.42
1:C:214:PHE:CE1	1:C:398:ARG:HD2	2.54	0.42
1:C:34:ARG:HH11	1:C:34:ARG:HG3	1.83	0.42
1:D:49:GLY:HA2	3:D:805:EDO:H12	2.00	0.42
1:C:359:LEU:HD12	1:C:373:THR:HA	2.02	0.42
1:A:361:GLU:O	1:A:362:ASP:HB2	2.20	0.42
1:B:61:LYS:HE3	1:B:317:GLN:OE1	2.20	0.42
1:C:86:TYR:C	1:C:86:TYR:CD2	2.92	0.42
1:B:390:CYS:SG	1:B:398:ARG:HD3	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ASN:HD22	1:C:319:ASN:HA	1.68	0.42
1:A:74:SER:O	1:A:302:PRO:HD2	2.20	0.42
1:A:347:ASP:O	1:A:357:ILE:HA	2.19	0.42
1:A:303:ILE:HD12	1:A:303:ILE:H	1.85	0.42
1:D:86:TYR:CD2	1:D:107:LEU:HD12	2.55	0.42
3:A:808:EDO:C1	1:B:81:LEU:HD12	2.50	0.42
1:D:332:LYS:HG3	1:D:348:VAL:HG12	2.00	0.42
1:A:224:ARG:HD2	5:A:914:HOH:O	2.20	0.42
1:C:22:ILE:HB	1:D:80:VAL:HA	2.02	0.42
1:A:76:THR:O	1:B:49:GLY:HA2	2.19	0.42
1:C:364:ASP:C	1:C:366:ASN:H	2.23	0.42
1:D:322:GLN:NE2	1:D:322:GLN:HA	2.34	0.42
1:B:357:ILE:HD11	1:B:397:LEU:HD12	2.02	0.42
1:D:422:ASP:O	1:D:426:GLN:HG3	2.20	0.42
1:B:121:ILE:HD13	1:B:286:MET:HE3	2.02	0.42
1:D:226:ARG:HG2	1:D:259:VAL:HG22	2.01	0.42
1:C:291:PRO:HA	1:D:17:ARG:O	2.20	0.42
1:C:228:LEU:HD23	1:C:228:LEU:C	2.41	0.41
1:B:59:HIS:CE1	1:B:61:LYS:HB2	2.56	0.41
1:C:73:LEU:C	1:C:73:LEU:HD12	2.40	0.41
1:D:191:PHE:HA	1:D:195:ALA:O	2.20	0.41
1:A:303:ILE:HD12	1:A:303:ILE:N	2.35	0.41
1:B:281:GLY:O	1:B:282:ARG:C	2.58	0.41
1:B:357:ILE:O	1:B:357:ILE:HG13	2.21	0.41
1:D:152:VAL:HG13	1:D:156:SER:HB2	2.03	0.41
1:C:17:ARG:HH12	1:D:290:ALA:HA	1.84	0.41
1:A:251:LEU:HD12	1:A:251:LEU:HA	1.91	0.41
1:D:357:ILE:HD11	1:D:397:LEU:HD12	2.02	0.41
1:D:331:LEU:O	1:D:335:LEU:HG	2.21	0.41
1:B:156:SER:HA	1:B:159:MET:HE3	1.99	0.41
1:A:364:ASP:O	1:A:366:ASN:N	2.42	0.41
1:B:401:VAL:HG21	1:B:405:ILE:HD12	2.02	0.41
1:A:348:VAL:HG22	1:A:357:ILE:HG22	2.03	0.41
1:D:307:ALA:O	1:D:311:VAL:HG23	2.20	0.41
1:A:32:ASN:C	1:A:32:ASN:HD22	2.24	0.41
1:A:87:LEU:HD21	1:B:10:ARG:HB2	2.01	0.41
1:C:74:SER:O	1:C:302:PRO:HD2	2.20	0.41
1:C:348:VAL:HG22	1:C:357:ILE:CG2	2.42	0.41
1:D:76:THR:O	1:D:77:CYS:CB	2.69	0.41
1:B:335:LEU:HD13	1:B:357:ILE:CG2	2.51	0.41
1:C:389:SER:HA	1:C:396:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASN:HA	1:A:154:PRO:HA	1.89	0.41
1:B:151:LYS:HZ2	1:D:192:LYS:HZ3	1.68	0.41
1:C:32:ASN:ND2	1:C:32:ASN:C	2.73	0.41
1:C:307:ALA:O	1:C:311:VAL:HG23	2.20	0.41
1:B:313:LYS:O	1:B:317:GLN:HG2	2.21	0.41
1:D:332:LYS:O	1:D:336:LEU:HG	2.21	0.41
1:B:162:MET:HB3	1:B:163:PRO:CD	2.51	0.41
1:A:51:ALA:HB2	1:A:400:LEU:HD22	2.03	0.41
1:B:162:MET:HB3	1:B:163:PRO:HD2	2.03	0.41
1:B:11:ARG:NH1	5:B:920:HOH:O	2.54	0.41
1:D:246:GLY:HA2	1:D:250:THR:O	2.20	0.41
1:B:73:LEU:HD12	1:B:73:LEU:C	2.42	0.41
1:D:276:LEU:HB2	1:D:304:ALA:HB1	2.03	0.41
1:D:73:LEU:HD12	1:D:73:LEU:C	2.41	0.40
1:C:252:PHE:O	1:C:255:GLU:HG3	2.21	0.40
1:B:43:TYR:CD1	1:B:43:TYR:N	2.89	0.40
1:C:330:LYS:NZ	1:C:407:ASP:OD1	2.53	0.40
1:C:209:GLN:O	1:C:214:PHE:HA	2.21	0.40
1:D:351:LEU:HA	1:D:351:LEU:HD23	1.97	0.40
1:D:274:PHE:HA	1:D:275:PRO:HD3	1.91	0.40
1:A:59:HIS:HE1	1:A:61:LYS:HG2	1.86	0.40
1:B:364:ASP:OD1	1:B:367:LYS:HG3	2.21	0.40
1:A:379:ARG:HE	1:A:424:ALA:HB2	1.86	0.40
1:D:315:PHE:CD2	1:D:320:LEU:HB2	2.56	0.40
1:C:357:ILE:HD11	1:C:397:LEU:HD12	2.02	0.40
1:C:86:TYR:C	1:C:86:TYR:HD2	2.25	0.40
1:C:251:LEU:HA	1:C:251:LEU:HD12	1.94	0.40
1:D:119:VAL:O	1:D:123:ARG:HG3	2.21	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	424/426 (100%)	395 (93%)	23 (5%)	6 (1%)	14	23
1	B	423/426 (99%)	393 (93%)	26 (6%)	4 (1%)	21	37
1	C	423/426 (99%)	394 (93%)	26 (6%)	3 (1%)	26	45
1	D	424/426 (100%)	391 (92%)	30 (7%)	3 (1%)	26	45
All	All	1694/1704 (99%)	1573 (93%)	105 (6%)	16 (1%)	21	37

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	HIS
1	B	155	TYR
1	B	365	HIS
1	D	50	ILE
1	B	267	ALA
1	A	50	ILE
1	A	77	CYS
1	A	366	ASN
1	B	50	ILE
1	C	275	PRO
1	D	267	ALA
1	C	267	ALA
1	D	108	VAL
1	A	275	PRO
1	C	50	ILE
1	A	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	330/330 (100%)	324 (98%)	6 (2%)	66	87
1	B	329/330 (100%)	325 (99%)	4 (1%)	78	92
1	C	329/330 (100%)	321 (98%)	8 (2%)	57	82
1	D	330/330 (100%)	323 (98%)	7 (2%)	61	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1318/1320 (100%)	1293 (98%)	25 (2%)	65 86

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	86	TYR
1	A	319	ASN
1	A	354	MET
1	A	362	ASP
1	A	366	ASN
1	B	32	ASN
1	B	154	PRO
1	B	415	GLU
1	B	426	GLN
1	C	32	ASN
1	C	86	TYR
1	C	163	PRO
1	C	319	ASN
1	C	351	LEU
1	C	362	ASP
1	C	394	TYR
1	C	415	GLU
1	D	32	ASN
1	D	86	TYR
1	D	89	LEU
1	D	154	PRO
1	D	259	VAL
1	D	319	ASN
1	D	394	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	9	GLN
1	A	13	GLN
1	A	32	ASN
1	A	94	ASN
1	A	317	GLN
1	A	319	ASN

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Mol	Chain	Res	Type
1	A	329	GLN
1	A	342	HIS
1	A	366	ASN
1	B	32	ASN
1	B	94	ASN
1	B	242	GLN
1	B	366	ASN
1	B	426	GLN
1	C	32	ASN
1	C	94	ASN
1	C	317	GLN
1	C	319	ASN
1	C	365	HIS
1	D	32	ASN
1	D	94	ASN
1	D	242	GLN
1	D	319	ASN
1	D	322	GLN
1	D	365	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

32 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	701	-	4,4,4	3.29	2 (50%)	6,6,6	0.97	0
2	SO4	A	707	-	4,4,4	3.27	2 (50%)	6,6,6	0.94	0
2	SO4	A	712	-	4,4,4	3.23	2 (50%)	6,6,6	0.95	0
4	PMP	A	750	-	16,16,16	5.57	4 (25%)	20,23,23	1.52	1 (5%)
3	EDO	A	808	-	3,3,3	0.54	0	2,2,2	0.39	0
3	EDO	A	810	-	3,3,3	0.55	0	2,2,2	0.43	0
3	EDO	A	813	-	3,3,3	0.55	0	2,2,2	0.46	0
2	SO4	B	702	-	4,4,4	3.33	2 (50%)	6,6,6	0.94	0
2	SO4	B	703	-	4,4,4	3.24	2 (50%)	6,6,6	0.98	0
2	SO4	B	708	-	4,4,4	3.27	2 (50%)	6,6,6	0.96	0
2	SO4	B	713	-	4,4,4	3.27	2 (50%)	6,6,6	0.94	0
4	PMP	B	751	-	16,16,16	5.66	5 (31%)	20,23,23	1.64	4 (20%)
3	EDO	B	801	-	3,3,3	0.58	0	2,2,2	0.37	0
3	EDO	B	802	-	3,3,3	0.62	0	2,2,2	0.41	0
3	EDO	B	804	-	3,3,3	0.59	0	2,2,2	0.43	0
2	SO4	C	704	-	4,4,4	3.30	2 (50%)	6,6,6	0.94	0
2	SO4	C	710	-	4,4,4	3.27	2 (50%)	6,6,6	0.98	0
2	SO4	C	714	-	4,4,4	3.28	2 (50%)	6,6,6	0.98	0
4	PMP	C	752	-	16,16,16	5.77	4 (25%)	20,23,23	1.54	1 (5%)
3	EDO	C	803	-	3,3,3	0.57	0	2,2,2	0.42	0
3	EDO	C	809	-	3,3,3	0.56	0	2,2,2	0.38	0
3	EDO	C	811	-	3,3,3	0.59	0	2,2,2	0.46	0
2	SO4	D	705	-	4,4,4	3.28	2 (50%)	6,6,6	0.96	0
2	SO4	D	706	-	4,4,4	3.25	2 (50%)	6,6,6	0.99	0
2	SO4	D	709	-	4,4,4	3.29	2 (50%)	6,6,6	0.94	0
2	SO4	D	711	-	4,4,4	3.27	2 (50%)	6,6,6	0.97	0
2	SO4	D	715	-	4,4,4	3.30	2 (50%)	6,6,6	0.95	0
4	PMP	D	753	-	16,16,16	5.46	5 (31%)	20,23,23	1.54	1 (5%)
3	EDO	D	805	-	3,3,3	0.51	0	2,2,2	0.45	0
3	EDO	D	806	-	3,3,3	0.58	0	2,2,2	0.44	0
3	EDO	D	807	-	3,3,3	0.52	0	2,2,2	0.46	0
3	EDO	D	812	-	3,3,3	0.49	0	2,2,2	0.50	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. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	701	-	-	0/0/0/0	0/0/0/0
2	SO4	A	707	-	-	0/0/0/0	0/0/0/0
2	SO4	A	712	-	-	0/0/0/0	0/0/0/0
4	PMP	A	750	-	-	0/8/8/8	0/1/1/1
3	EDO	A	808	-	-	0/1/1/1	0/0/0/0
3	EDO	A	810	-	-	0/1/1/1	0/0/0/0
3	EDO	A	813	-	-	0/1/1/1	0/0/0/0
2	SO4	B	702	-	-	0/0/0/0	0/0/0/0
2	SO4	B	703	-	-	0/0/0/0	0/0/0/0
2	SO4	B	708	-	-	0/0/0/0	0/0/0/0
2	SO4	B	713	-	-	0/0/0/0	0/0/0/0
4	PMP	B	751	-	-	0/8/8/8	0/1/1/1
3	EDO	B	801	-	-	0/1/1/1	0/0/0/0
3	EDO	B	802	-	-	0/1/1/1	0/0/0/0
3	EDO	B	804	-	-	0/1/1/1	0/0/0/0
2	SO4	C	704	-	-	0/0/0/0	0/0/0/0
2	SO4	C	710	-	-	0/0/0/0	0/0/0/0
2	SO4	C	714	-	-	0/0/0/0	0/0/0/0
4	PMP	C	752	-	-	0/8/8/8	0/1/1/1
3	EDO	C	803	-	-	0/1/1/1	0/0/0/0
3	EDO	C	809	-	-	0/1/1/1	0/0/0/0
3	EDO	C	811	-	-	0/1/1/1	0/0/0/0
2	SO4	D	705	-	-	0/0/0/0	0/0/0/0
2	SO4	D	706	-	-	0/0/0/0	0/0/0/0
2	SO4	D	709	-	-	0/0/0/0	0/0/0/0
2	SO4	D	711	-	-	0/0/0/0	0/0/0/0
2	SO4	D	715	-	-	0/0/0/0	0/0/0/0
4	PMP	D	753	-	-	0/8/8/8	0/1/1/1
3	EDO	D	805	-	-	0/1/1/1	0/0/0/0
3	EDO	D	806	-	-	0/1/1/1	0/0/0/0
3	EDO	D	807	-	-	0/1/1/1	0/0/0/0
3	EDO	D	812	-	-	0/1/1/1	0/0/0/0

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	715	SO4	O3-S	-4.67	1.30	1.47
2	B	713	SO4	O3-S	-4.67	1.30	1.47
2	A	712	SO4	O3-S	-4.65	1.30	1.47
2	D	709	SO4	O3-S	-4.58	1.30	1.47
2	C	714	SO4	O3-S	-4.57	1.30	1.47
2	B	702	SO4	O3-S	-4.56	1.31	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	708	SO4	O3-S	-4.54	1.31	1.47
2	C	704	SO4	O3-S	-4.54	1.31	1.47
2	A	707	SO4	O3-S	-4.53	1.31	1.47
2	C	710	SO4	O3-S	-4.52	1.31	1.47
2	D	711	SO4	O3-S	-4.52	1.31	1.47
2	D	706	SO4	O3-S	-4.51	1.31	1.47
2	A	701	SO4	O3-S	-4.48	1.31	1.47
2	D	705	SO4	O3-S	-4.47	1.31	1.47
2	B	703	SO4	O3-S	-4.41	1.31	1.47
4	D	753	PMP	P-O3P	-2.05	1.47	1.54
4	B	751	PMP	C2A-C2	2.09	1.54	1.50
4	C	752	PMP	C2-N1	3.33	1.41	1.34
4	A	750	PMP	C2-N1	3.37	1.41	1.34
4	B	751	PMP	C2-N1	3.54	1.41	1.34
4	D	753	PMP	C2-N1	3.59	1.41	1.34
4	A	750	PMP	C6-N1	4.26	1.43	1.34
2	A	712	SO4	O1-S	4.39	1.62	1.47
2	B	713	SO4	O1-S	4.49	1.62	1.47
4	C	752	PMP	C6-N1	4.52	1.44	1.34
2	D	706	SO4	O1-S	4.57	1.62	1.47
2	C	714	SO4	O1-S	4.58	1.62	1.47
2	D	715	SO4	O1-S	4.58	1.62	1.47
2	A	707	SO4	O1-S	4.62	1.63	1.47
2	B	708	SO4	O1-S	4.62	1.63	1.47
2	C	710	SO4	O1-S	4.64	1.63	1.47
2	D	711	SO4	O1-S	4.65	1.63	1.47
2	D	709	SO4	O1-S	4.65	1.63	1.47
2	B	703	SO4	O1-S	4.65	1.63	1.47
2	C	704	SO4	O1-S	4.70	1.63	1.47
2	A	701	SO4	O1-S	4.70	1.63	1.47
2	D	705	SO4	O1-S	4.71	1.63	1.47
2	B	702	SO4	O1-S	4.76	1.63	1.47
4	D	753	PMP	C6-N1	4.77	1.44	1.34
4	B	751	PMP	C6-N1	5.00	1.45	1.34
4	B	751	PMP	C5-C4	13.52	1.59	1.40
4	C	752	PMP	C5-C4	13.62	1.59	1.40
4	A	750	PMP	C5-C4	13.63	1.59	1.40
4	D	753	PMP	C5-C4	13.80	1.60	1.40
4	D	753	PMP	C3-C2	15.28	1.51	1.40
4	A	750	PMP	C3-C2	16.41	1.52	1.40
4	B	751	PMP	C3-C2	16.62	1.52	1.40
4	C	752	PMP	C3-C2	17.39	1.52	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	751	PMP	O4P-P-O1P	-2.17	101.61	107.14
4	B	751	PMP	C3-C2-N1	-2.04	117.80	120.61
4	B	751	PMP	O4P-C5A-C5	2.38	112.93	108.99
4	D	753	PMP	C2A-C2-C3	4.18	126.08	121.04
4	C	752	PMP	C2A-C2-C3	4.45	126.41	121.04
4	A	750	PMP	C2A-C2-C3	4.68	126.69	121.04
4	B	751	PMP	C2A-C2-C3	4.69	126.69	121.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	712	SO4	1	0
4	A	750	PMP	1	0
3	A	808	EDO	2	0
3	A	810	EDO	1	0
4	B	751	PMP	1	0
3	B	801	EDO	3	0
3	B	804	EDO	1	0
2	C	714	SO4	1	0
3	C	803	EDO	1	0
4	D	753	PMP	1	0
3	D	805	EDO	4	0
3	D	812	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	425/426 (99%)	-0.19	11 (2%) 59 64	18, 32, 57, 86	0
1	B	425/426 (99%)	-0.13	15 (3%) 48 53	17, 32, 69, 97	0
1	C	425/426 (99%)	0.06	23 (5%) 29 34	17, 39, 79, 100	0
1	D	425/426 (99%)	-0.10	16 (3%) 44 50	16, 31, 66, 94	0
All	All	1700/1704 (99%)	-0.09	65 (3%) 44 50	16, 33, 70, 100	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	426	GLN	6.1
1	C	362	ASP	5.7
1	B	426	GLN	5.4
1	D	365	HIS	4.6
1	D	360	PHE	4.4
1	D	366	ASN	4.3
1	C	363	GLY	4.3
1	D	426	GLN	4.3
1	A	426	GLN	4.0
1	C	424	ALA	4.0
1	A	362	ASP	3.7
1	A	425	LYS	3.6
1	B	424	ALA	3.6
1	C	341	LYS	3.6
1	D	362	ASP	3.6
1	D	363	GLY	3.5
1	D	364	ASP	3.4
1	B	362	ASP	3.4
1	C	360	PHE	3.3
1	C	364	ASP	3.3
1	A	368	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	368	PRO	3.1
1	A	361	GLU	3.1
1	D	393	TYR	3.1
1	B	363	GLY	3.0
1	B	343	PRO	3.0
1	A	424	ALA	3.0
1	C	343	PRO	2.9
1	C	425	LYS	2.9
1	C	366	ASN	2.9
1	C	367	LYS	2.9
1	A	360	PHE	2.9
1	B	365	HIS	2.9
1	B	341	LYS	2.9
1	A	365	HIS	2.8
1	B	367	LYS	2.8
1	B	368	PRO	2.8
1	C	361	GLU	2.8
1	C	339	ALA	2.8
1	C	421	PHE	2.7
1	B	425	LYS	2.7
1	D	425	LYS	2.7
1	A	2	ASN	2.6
1	A	364	ASP	2.6
1	C	365	HIS	2.6
1	D	341	LYS	2.6
1	B	421	PHE	2.6
1	C	338	ILE	2.5
1	C	376	ILE	2.5
1	C	380	ALA	2.5
1	A	366	ASN	2.4
1	C	415	GLU	2.4
1	C	422	ASP	2.3
1	D	361	GLU	2.3
1	D	340	GLU	2.3
1	D	114	ALA	2.2
1	C	371	LYS	2.2
1	B	366	ASN	2.2
1	D	112[A]	SER	2.1
1	B	344	GLU	2.1
1	D	110	THR	2.1
1	D	421	PHE	2.1
1	B	339	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	335	LEU	2.0
1	B	340	GLU	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	EDO	C	803	4/4	0.89	0.28	9.13	50,50,51,55	0
2	SO4	A	712	5/5	0.75	0.28	7.05	120,120,120,120	0
3	EDO	B	804	4/4	0.90	0.26	6.76	50,50,51,54	0
3	EDO	A	808	4/4	0.97	0.22	5.85	51,52,52,53	0
3	EDO	D	807	4/4	0.95	0.23	5.76	53,54,54,56	0
3	EDO	C	809	4/4	0.95	0.23	4.15	53,55,56,57	0
3	EDO	B	801	4/4	0.93	0.20	3.23	47,47,48,48	0
3	EDO	D	806	4/4	0.97	0.23	2.96	52,55,55,57	0
3	EDO	A	810	4/4	0.91	0.20	2.93	53,56,57,57	0
2	SO4	B	713	5/5	0.91	0.28	2.55	117,117,118,118	0
3	EDO	D	812	4/4	0.92	0.16	2.17	33,34,37,37	0
2	SO4	D	715	5/5	0.92	0.24	2.13	119,120,120,120	0
3	EDO	A	813	4/4	0.95	0.18	1.76	49,50,51,52	0
3	EDO	D	805	4/4	0.95	0.18	1.52	42,42,43,45	0
3	EDO	C	811	4/4	0.95	0.15	1.49	31,32,33,34	0
2	SO4	C	714	5/5	0.91	0.18	0.85	106,107,107,107	0
4	PMP	C	752	16/16	0.97	0.20	0.33	25,31,36,37	0
4	PMP	A	750	16/16	0.98	0.18	0.33	24,28,32,35	0
4	PMP	B	751	16/16	0.98	0.20	0.21	18,28,32,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	PMP	D	753	16/16	0.98	0.21	0.05	21,24,32,34	0
3	EDO	B	802	4/4	0.91	0.14	-0.26	38,41,43,43	0
2	SO4	B	702	5/5	0.85	0.17	-	94,94,95,95	0
2	SO4	D	711	5/5	0.66	0.47	-	130,130,130,131	0
2	SO4	D	706	5/5	0.86	0.16	-	110,110,110,110	0
2	SO4	B	708	5/5	0.86	0.18	-	106,107,107,107	0
2	SO4	B	703	5/5	0.88	0.27	-	96,97,97,98	0
2	SO4	C	710	5/5	0.96	0.23	-	94,94,95,95	0
2	SO4	D	705	5/5	0.93	0.23	-	88,88,88,88	0
2	SO4	A	707	5/5	0.87	0.17	-	113,113,114,114	0
2	SO4	A	701	5/5	0.90	0.20	-	114,114,114,115	0
2	SO4	D	709	5/5	0.91	0.23	-	101,101,102,102	0
2	SO4	C	704	5/5	0.86	0.22	-	100,100,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.