



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:24 am BST

PDB ID : 4BOF
Title : Crystal structure of arginine deiminase from group A streptococcus
Authors : Henningham, A.; Ericsson, D.J.; Langer, K.; Casey, L.; Jovcevski, B.; Chhatwal, G.S.; Aquilina, J.A.; Batzloff, M.R.; Kobe, B.; Walker, M.J.
Deposited on : 2013-05-20
Resolution : 2.48 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

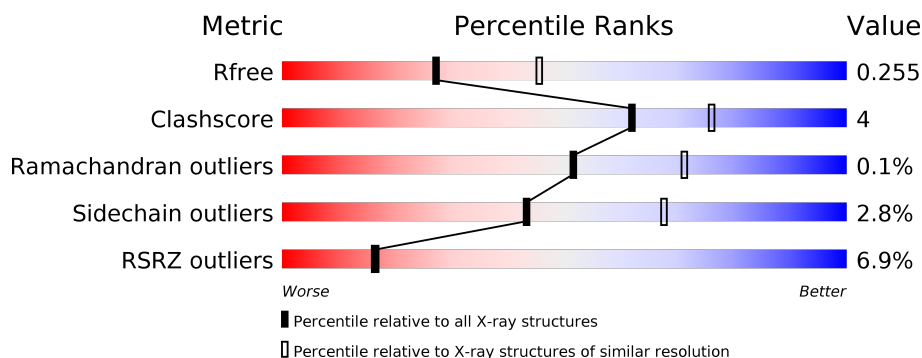
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



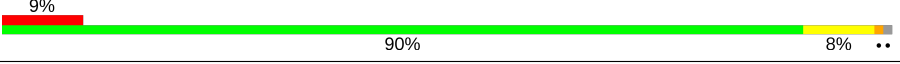

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	411	<div> <div>3%</div> <div>87%</div> <div>11%</div> </div>
1	B	411	<div> <div>5%</div> <div>91%</div> <div>9%</div> </div>
1	C	411	<div> <div>2%</div> <div>89%</div> <div>9%</div> </div>
1	D	411	<div> <div>3%</div> <div>89%</div> <div>10%</div> </div>
1	E	411	<div> <div>18%</div> <div>88%</div> <div>11%</div> </div>
1	F	411	<div> <div>2%</div> <div>88%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	411	
1	H	411	

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	420	-	-	X	-
2	SO4	B	420	-	-	X	-
2	SO4	C	420	-	-	X	-
2	SO4	D	420	-	-	X	-
2	SO4	E	420	-	-	X	-
2	SO4	F	420	-	-	X	-
2	SO4	G	420	-	-	X	-
3	PGE	A	422	-	-	X	-
4	PG4	F	422	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26319 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 ARGININE DEIMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3237	2055	547	623	12			
1	B	411	Total	C	N	O	S	0	0	0
			3257	2067	550	627	13			
1	C	409	Total	C	N	O	S	0	0	0
			3242	2058	548	624	12			
1	D	409	Total	C	N	O	S	0	0	0
			3242	2058	548	624	12			
1	E	406	Total	C	N	O	S	0	0	0
			3221	2046	544	619	12			
1	F	409	Total	C	N	O	S	0	0	0
			3242	2058	548	624	12			
1	G	408	Total	C	N	O	S	0	0	0
			3237	2055	547	623	12			
1	H	408	Total	C	N	O	S	0	0	0
			3237	2055	547	623	12			

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



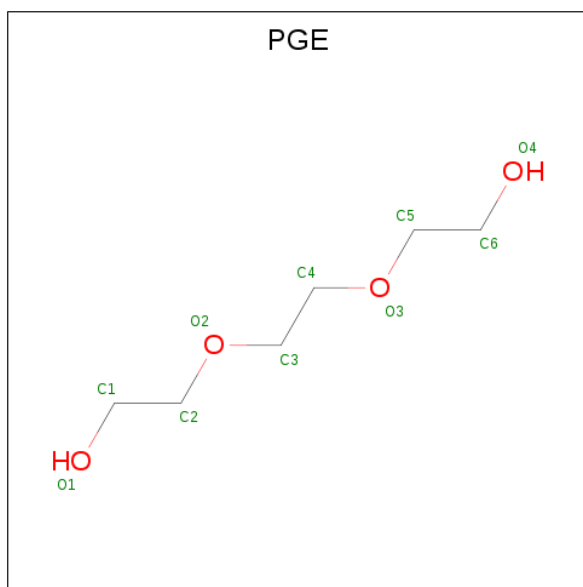
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total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

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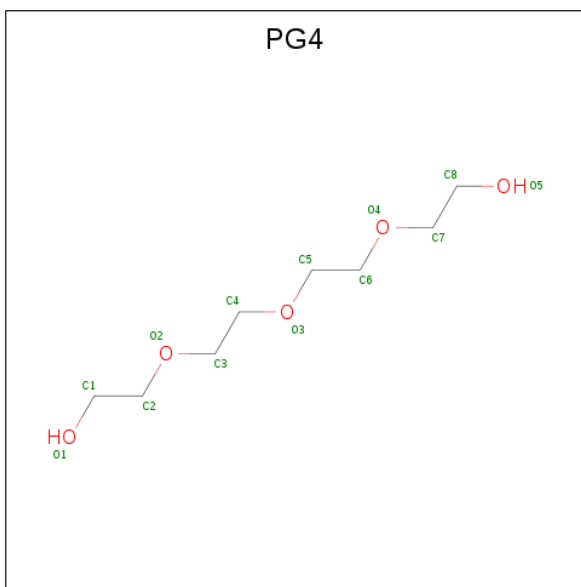
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			13	8	5		

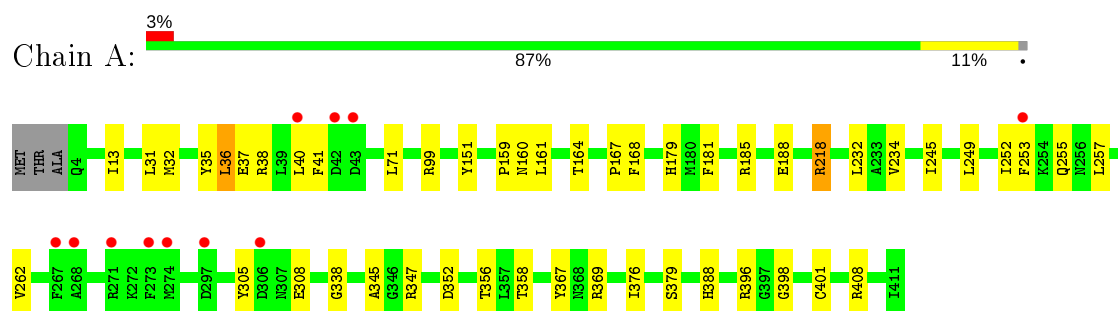
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total	O	0	0
			67	67		
5	B	20	Total	O	0	0
			20	20		
5	C	49	Total	O	0	0
			49	49		
5	D	41	Total	O	0	0
			41	41		
5	E	7	Total	O	0	0
			7	7		
5	F	62	Total	O	0	0
			62	62		
5	G	20	Total	O	0	0
			20	20		
5	H	25	Total	O	0	0
			25	25		

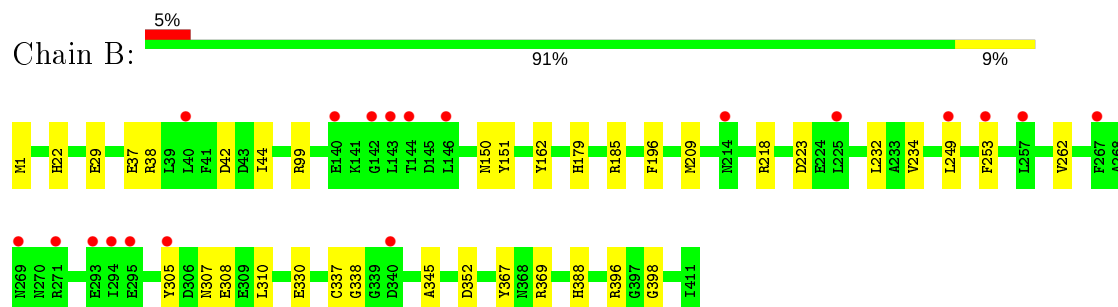
3 Residue-property plots [i](#)

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

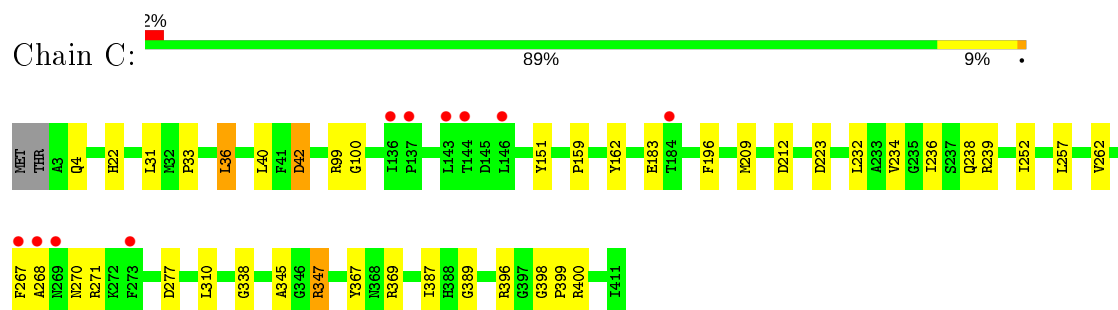
• Molecule 1: ARGININE DEIMINASE



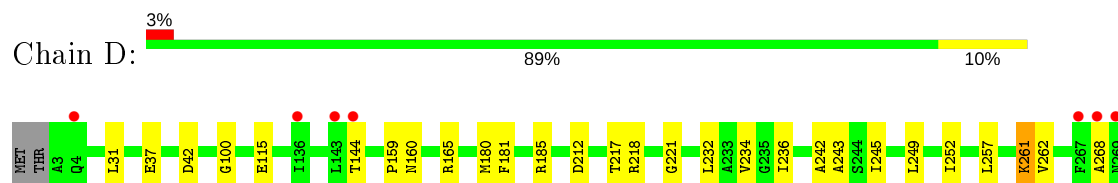
• Molecule 1: ARGININE DEIMINASE

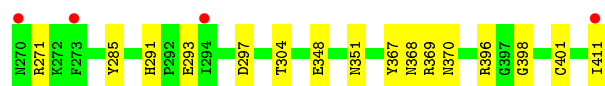


• Molecule 1: ARGININE DEIMINASE

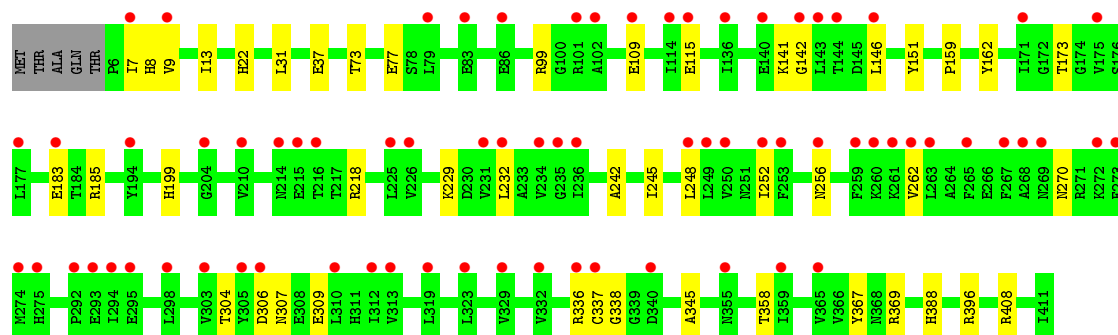
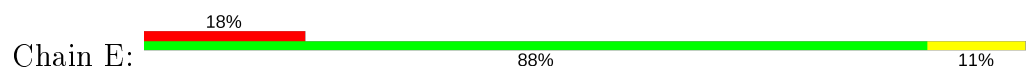


• Molecule 1: ARGININE DEIMINASE

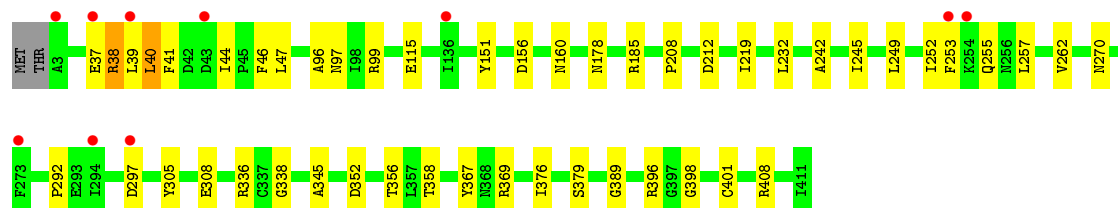
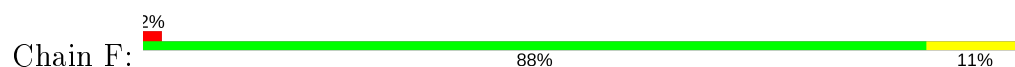




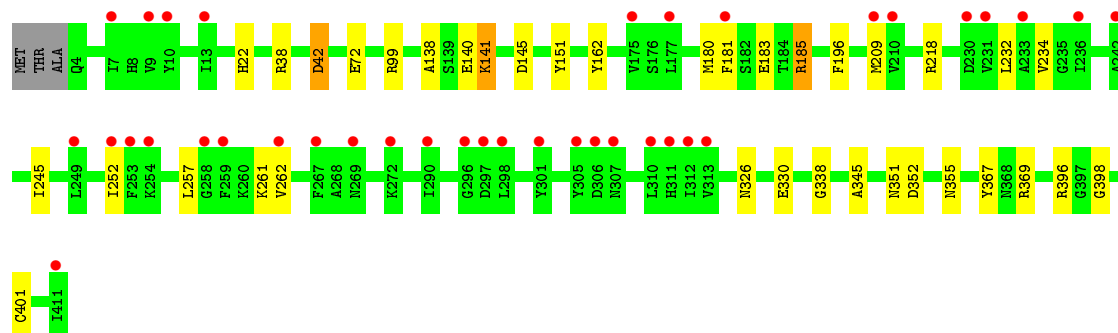
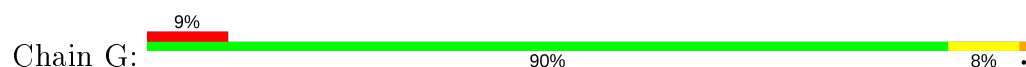
• Molecule 1: ARGININE DEIMINASE



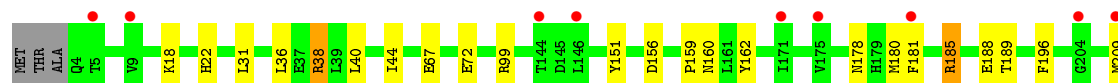
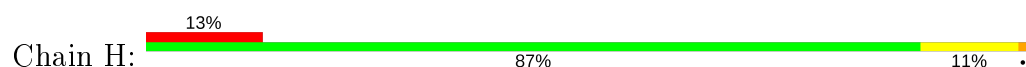
• Molecule 1: ARGININE DEIMINASE

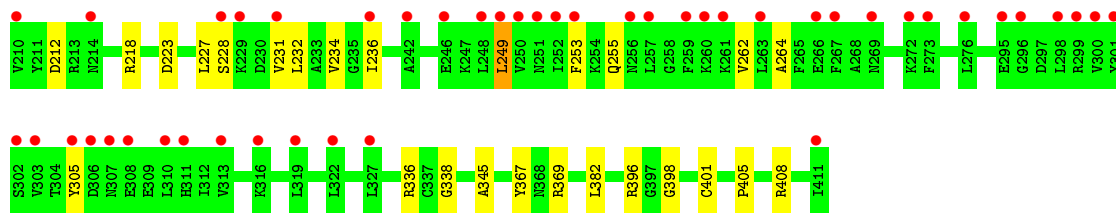


• Molecule 1: ARGININE DEIMINASE



• Molecule 1: ARGININE DEIMINASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.91Å 92.74Å 120.97Å 96.15° 90.27° 100.13°	Depositor
Resolution (Å)	36.31 – 2.48 61.60 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.31-2.48) 99.3 (61.60-2.48)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.211 , 0.244 0.222 , 0.255	Depositor DCC
R_{free} test set	6579 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26319	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, PGE, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/3296	0.70	0/4457
1	B	0.47	0/3316	0.65	0/4484
1	C	0.52	0/3301	0.69	1/4464 (0.0%)
1	D	0.52	0/3301	0.68	0/4464
1	E	0.47	0/3280	0.66	0/4434
1	F	0.54	0/3301	0.70	0/4464
1	G	0.48	0/3296	0.65	0/4457
1	H	0.47	0/3296	0.65	0/4457
All	All	0.50	0/26387	0.67	1/35681 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	GLN	C-N-CA	5.53	135.52	121.70

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	3237	0	3231	48	0
1	B	3257	0	3255	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3242	0	3236	25	0
1	D	3242	0	3236	23	0
1	E	3221	0	3217	22	0
1	F	3242	0	3236	41	0
1	G	3237	0	3231	25	0
1	H	3237	0	3231	29	0
2	A	10	0	0	2	0
2	B	10	0	0	3	0
2	C	10	0	0	4	0
2	D	10	0	0	2	0
2	E	10	0	0	3	0
2	F	10	0	0	4	0
2	G	10	0	0	3	0
2	H	10	0	0	1	0
3	A	10	0	14	20	0
3	F	10	0	14	4	0
4	F	13	0	18	14	0
5	A	67	0	0	3	0
5	B	20	0	0	0	0
5	C	49	0	0	1	0
5	D	41	0	0	1	0
5	E	7	0	0	0	0
5	F	62	0	0	2	0
5	G	20	0	0	0	0
5	H	25	0	0	2	0
All	All	26319	0	25919	226	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 4.

All (226) 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:H:369:ARG:HD2	2:H:420:SO4:O3	1.56	1.03
1:A:167:PRO:HG2	3:A:422:PGE:H52	1.47	0.97
1:A:249:LEU:HD22	1:A:262:VAL:HG21	1.46	0.95
1:G:369:ARG:HD2	2:G:420:SO4:O3	1.67	0.95
1:F:249:LEU:HD22	1:F:262:VAL:HG21	1.48	0.93
4:F:422:PG4:H21	1:G:369:ARG:HH21	1.32	0.93
1:A:167:PRO:HB2	3:A:422:PGE:H22	1.50	0.91
1:A:245:ILE:O	1:A:249:LEU:HG	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:GLY:O	1:E:146:LEU:HD13	1.76	0.85
1:A:188:GLU:OE1	3:A:422:PGE:H62	1.75	0.85
1:B:179:HIS:HD2	1:B:218:ARG:HD3	1.40	0.83
1:C:389:GLY:N	2:C:420:SO4:O3	2.09	0.83
1:F:358:THR:O	1:F:408:ARG:NH2	2.11	0.83
1:F:44:ILE:O	4:F:422:PG4:H12	1.80	0.81
1:C:267:PHE:HB2	1:C:270:ASN:HD22	1.46	0.80
1:A:164:THR:HA	3:A:422:PGE:H3	1.66	0.78
1:B:179:HIS:CD2	1:B:218:ARG:HD3	2.21	0.76
1:F:369:ARG:NH1	2:F:420:SO4:O4	2.18	0.75
1:A:168:PHE:CE2	3:A:422:PGE:H2	2.22	0.75
1:F:46:PHE:HD1	4:F:422:PG4:H51	1.51	0.74
1:A:167:PRO:CG	3:A:422:PGE:H52	2.16	0.74
1:D:369:ARG:HB3	2:D:420:SO4:O2	1.88	0.74
4:F:422:PG4:H31	1:G:351:ASN:ND2	2.04	0.72
1:A:388:HIS:HA	2:A:420:SO4:O1	1.90	0.72
1:B:369:ARG:HB3	2:B:420:SO4:O3	1.90	0.72
1:E:141:LYS:HB3	1:E:146:LEU:HD12	1.73	0.71
1:C:369:ARG:NH1	2:C:420:SO4:O2	2.25	0.69
1:F:245:ILE:O	1:F:249:LEU:HG	1.91	0.69
1:H:180:MET:HE3	1:H:185:ARG:HG2	1.75	0.67
1:F:47:LEU:H	4:F:422:PG4:H62	1.58	0.67
1:A:356:THR:HA	5:A:2060:HOH:O	1.96	0.66
1:F:46:PHE:CD1	4:F:422:PG4:H51	2.31	0.65
1:H:181:PHE:HA	1:H:218:ARG:HD2	1.79	0.65
1:D:252:ILE:HG23	1:D:257:LEU:HB2	1.79	0.65
1:D:236:ILE:HG22	1:D:268:ALA:HB2	1.80	0.64
1:F:356:THR:HA	5:F:2051:HOH:O	1.96	0.64
1:C:196:PHE:HB3	1:C:209:MET:HE3	1.80	0.63
1:A:358:THR:O	1:A:408:ARG:NH2	2.26	0.63
1:C:196:PHE:HB3	1:C:209:MET:CE	2.29	0.63
1:C:252:ILE:HG23	1:C:257:LEU:HB2	1.81	0.62
1:F:369:ARG:N	2:F:420:SO4:O2	2.27	0.62
1:E:141:LYS:HB3	1:E:146:LEU:CD1	2.29	0.62
1:E:369:ARG:HB3	2:E:420:SO4:O1	1.99	0.62
1:A:167:PRO:HG2	3:A:422:PGE:C5	2.28	0.62
1:G:181:PHE:HA	1:G:218:ARG:HD2	1.82	0.62
1:A:167:PRO:HG2	3:A:422:PGE:H32	1.82	0.61
1:E:388:HIS:HA	2:E:420:SO4:O2	2.01	0.61
1:H:196:PHE:HB3	1:H:209:MET:CE	2.30	0.61
1:F:44:ILE:O	4:F:422:PG4:C1	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:422:PG4:H22	1:G:369:ARG:HE	1.66	0.61
1:D:291:HIS:CE1	1:D:293:GLU:HB2	2.37	0.60
1:G:196:PHE:HB3	1:G:209:MET:HE3	1.84	0.60
1:H:227:LEU:HB2	1:H:231:VAL:HG13	1.83	0.59
1:D:181:PHE:HA	1:D:218:ARG:HD2	1.82	0.59
1:F:292:PRO:HB3	1:F:336:ARG:HE	1.68	0.59
1:G:138:ALA:HA	1:G:141:LYS:HD3	1.84	0.59
1:B:196:PHE:HB3	1:B:209:MET:CE	2.32	0.59
1:A:168:PHE:CD2	3:A:422:PGE:H2	2.38	0.59
1:D:348:GLU:HG2	1:D:370:ASN:HD22	1.68	0.58
1:D:261:LYS:HG3	1:D:304:THR:HG22	1.83	0.58
1:G:22:HIS:HB3	1:G:162:TYR:HA	1.85	0.58
1:A:181:PHE:HA	1:A:218:ARG:HG2	1.84	0.58
1:B:196:PHE:HB3	1:B:209:MET:HE3	1.83	0.58
1:A:179:HIS:HD2	1:A:218:ARG:HG3	1.68	0.58
1:D:234:VAL:HG21	1:D:245:ILE:HG12	1.85	0.58
1:E:183:GLU:HG2	1:E:218:ARG:HH12	1.69	0.57
1:H:236:ILE:HD11	1:H:264:ALA:HB1	1.86	0.57
1:A:347:ARG:HG2	1:H:44:ILE:HG21	1.84	0.57
1:G:196:PHE:HB3	1:G:209:MET:CE	2.35	0.57
1:G:141:LYS:HG2	1:G:145:ASP:HB3	1.87	0.56
1:H:180:MET:CE	1:H:185:ARG:HG2	2.34	0.56
1:A:160:ASN:O	3:A:422:PGE:H6	2.06	0.56
1:C:369:ARG:HB3	2:C:420:SO4:O2	2.04	0.56
1:G:232:LEU:HB2	1:G:262:VAL:HG22	1.87	0.56
1:E:77:GLU:HB2	1:E:199:HIS:HE1	1.70	0.56
1:A:232:LEU:HB2	1:A:262:VAL:HG22	1.88	0.55
1:E:22:HIS:HB3	1:E:162:TYR:HA	1.88	0.55
1:G:180:MET:HE3	1:G:185:ARG:HG2	1.88	0.55
1:C:238:GLN:HG3	1:C:239:ARG:HG2	1.89	0.54
1:F:369:ARG:HD2	2:F:420:SO4:O4	2.06	0.54
1:H:40:LEU:O	5:H:2006:HOH:O	2.18	0.54
1:A:167:PRO:CB	3:A:422:PGE:H22	2.32	0.54
1:B:249:LEU:HD11	1:B:253:PHE:HE1	1.73	0.54
1:C:40:LEU:O	5:C:2010:HOH:O	2.18	0.54
1:A:188:GLU:OE1	3:A:422:PGE:C6	2.54	0.54
1:E:77:GLU:HB2	1:E:199:HIS:CE1	2.43	0.54
1:F:232:LEU:HB2	1:F:262:VAL:HG22	1.90	0.53
1:H:232:LEU:HB2	1:H:262:VAL:HG22	1.89	0.53
1:A:249:LEU:O	1:A:253:PHE:HD2	1.92	0.53
1:E:367:TYR:HB3	2:E:420:SO4:O3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ILE:O	4:F:422:PG4:C2	2.57	0.53
1:A:185:ARG:HH21	3:A:422:PGE:H62	1.73	0.53
1:B:232:LEU:HB2	1:B:262:VAL:HG22	1.89	0.53
1:C:277:ASP:OD2	1:C:400:ARG:NH1	2.42	0.53
1:B:44:ILE:HG21	1:C:347:ARG:HG2	1.91	0.52
1:A:161:LEU:HA	3:A:422:PGE:H5	1.92	0.52
1:D:232:LEU:HB2	1:D:262:VAL:HG22	1.90	0.52
1:C:236:ILE:HG22	1:C:268:ALA:HB2	1.91	0.52
1:H:22:HIS:HB3	1:H:162:TYR:HA	1.91	0.52
1:A:160:ASN:ND2	5:A:2011:HOH:O	2.36	0.51
1:H:249:LEU:O	1:H:253:PHE:HD1	1.91	0.51
1:F:389:GLY:N	2:F:420:SO4:O1	2.43	0.51
1:A:249:LEU:CD2	1:A:262:VAL:HG21	2.32	0.51
1:F:156:ASP:CB	3:F:423:PGE:H6	2.41	0.51
1:F:249:LEU:O	1:F:253:PHE:HD2	1.94	0.51
1:C:232:LEU:HB2	1:C:262:VAL:HG22	1.93	0.51
1:H:196:PHE:HB3	1:H:209:MET:HE3	1.92	0.50
1:D:242:ALA:HA	1:D:245:ILE:HD12	1.93	0.50
1:A:185:ARG:HH21	3:A:422:PGE:C6	2.25	0.50
1:F:252:ILE:HG23	1:F:257:LEU:HB2	1.94	0.50
1:G:234:VAL:HG21	1:G:245:ILE:HG23	1.94	0.50
1:B:99:ARG:HH22	1:B:151:TYR:HB3	1.77	0.50
1:G:369:ARG:NH1	2:G:420:SO4:O3	2.32	0.50
1:E:232:LEU:HB2	1:E:262:VAL:HG22	1.93	0.50
1:A:167:PRO:CG	3:A:422:PGE:H32	2.41	0.49
1:D:368:ASN:N	2:D:420:SO4:O1	2.45	0.49
1:F:249:LEU:CD2	1:F:262:VAL:HG21	2.33	0.49
4:F:422:PG4:H21	1:G:369:ARG:NH2	2.15	0.49
1:A:252:ILE:HG23	1:A:257:LEU:HB2	1.94	0.49
1:A:99:ARG:HH22	1:A:151:TYR:HB3	1.77	0.48
1:G:99:ARG:HH22	1:G:151:TYR:HB3	1.78	0.48
1:H:228:SER:OG	1:H:231:VAL:HG12	2.13	0.48
1:F:156:ASP:HB3	3:F:423:PGE:H6	1.94	0.48
1:G:38:ARG:NH2	1:G:151:TYR:OH	2.46	0.48
1:F:305:TYR:CE2	1:F:308:GLU:HA	2.48	0.48
1:F:99:ARG:HH22	1:F:151:TYR:HB3	1.77	0.48
1:H:99:ARG:HH22	1:H:151:TYR:HB3	1.79	0.48
1:B:249:LEU:CD1	1:B:253:PHE:HE1	2.26	0.48
1:H:196:PHE:HB3	1:H:209:MET:HE1	1.96	0.48
1:D:261:LYS:HG3	1:D:304:THR:CG2	2.44	0.47
1:D:351:ASN:HB2	1:D:370:ASN:HD21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:ARG:HH22	1:E:151:TYR:HB3	1.79	0.47
1:A:379:SER:HB2	1:F:376:ILE:HG13	1.95	0.47
1:C:99:ARG:HH22	1:C:151:TYR:HB3	1.78	0.47
1:G:42:ASP:OD1	1:G:396:ARG:HG2	2.14	0.47
1:A:367:TYR:CE2	1:A:398:GLY:HA2	2.50	0.47
1:F:338:GLY:HA3	1:F:345:ALA:HA	1.96	0.47
1:A:71:LEU:HD11	3:A:422:PGE:H12	1.96	0.47
1:B:305:TYR:HD1	1:B:310:LEU:HG	1.80	0.47
1:E:13:ILE:HG22	1:E:358:THR:HG21	1.97	0.47
1:E:338:GLY:HA3	1:E:345:ALA:HA	1.97	0.47
1:F:242:ALA:HA	1:F:245:ILE:HD12	1.96	0.47
1:A:379:SER:HB2	1:F:376:ILE:CG1	2.45	0.47
1:A:31:LEU:HD21	1:A:159:PRO:HG3	1.98	0.46
1:C:100:GLY:HA2	2:C:421:SO4:O1	2.16	0.46
1:H:38:ARG:NH2	1:H:156:ASP:OD2	2.49	0.46
1:C:223:ASP:O	1:C:234:VAL:HA	2.16	0.46
1:E:248:LEU:HG	1:E:252:ILE:HD12	1.98	0.46
1:F:249:LEU:O	1:F:253:PHE:CD2	2.68	0.46
1:E:77:GLU:CB	1:E:199:HIS:CE1	2.99	0.45
1:F:37:GLU:HG3	1:F:38:ARG:N	2.31	0.45
1:F:160:ASN:ND2	5:F:2013:HOH:O	2.42	0.45
1:F:367:TYR:CE2	1:F:398:GLY:HA2	2.52	0.45
1:H:338:GLY:HA3	1:H:345:ALA:HA	1.98	0.45
1:D:367:TYR:CE2	1:D:398:GLY:HA2	2.51	0.45
1:F:46:PHE:HA	4:F:422:PG4:H41	1.97	0.45
1:A:161:LEU:HA	3:A:422:PGE:C5	2.46	0.45
1:C:42:ASP:OD1	1:C:396:ARG:HG2	2.17	0.45
1:F:208:PRO:HB3	1:F:255:GLN:HG2	1.98	0.45
1:H:38:ARG:C	1:H:40:LEU:H	2.20	0.45
1:E:77:GLU:CB	1:E:199:HIS:HE1	2.30	0.45
1:G:261:LYS:NZ	1:G:326:ASN:HD21	2.15	0.45
1:G:369:ARG:N	2:G:420:SO4:O4	2.50	0.45
1:H:367:TYR:CE2	1:H:398:GLY:HA2	2.52	0.45
1:A:32:MET:O	1:A:36:LEU:HD13	2.16	0.44
1:B:367:TYR:CE2	1:B:398:GLY:HA2	2.53	0.44
1:E:9:VAL:HG22	1:E:408:ARG:HG3	1.98	0.44
1:F:96:ALA:O	3:F:423:PGE:H32	2.17	0.44
1:F:97:ASN:HD22	3:F:423:PGE:H4	1.82	0.44
1:A:249:LEU:O	1:A:253:PHE:CD2	2.69	0.44
1:H:223:ASP:O	1:H:234:VAL:HA	2.18	0.44
1:B:22:HIS:HB3	1:B:162:TYR:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ASP:O	1:B:234:VAL:HA	2.18	0.44
1:A:305:TYR:CE2	1:A:308:GLU:HA	2.53	0.44
1:B:338:GLY:HA3	1:B:345:ALA:HA	1.99	0.44
1:D:180:MET:HE3	1:D:185:ARG:HB3	2.00	0.44
1:D:100:GLY:HA2	1:D:144:THR:HG23	2.00	0.43
1:F:178:ASN:HB3	1:F:219:ILE:O	2.18	0.43
1:C:367:TYR:CE2	1:C:398:GLY:HA2	2.53	0.43
1:G:338:GLY:HA3	1:G:345:ALA:HA	2.00	0.43
1:C:33:PRO:HA	1:C:36:LEU:HD22	2.00	0.43
1:D:234:VAL:CG2	1:D:245:ILE:HG12	2.46	0.43
1:G:352:ASP:HB3	1:G:355:ASN:HB3	2.00	0.43
1:C:387:ILE:HD11	1:C:399:PRO:HG3	2.00	0.43
1:H:178:ASN:O	1:H:189:THR:HG21	2.19	0.43
1:H:253:PHE:CD2	1:H:305:TYR:HB3	2.54	0.43
1:A:161:LEU:HD23	3:A:422:PGE:H4	2.00	0.43
1:F:37:GLU:HG3	1:F:38:ARG:H	1.84	0.43
1:C:22:HIS:HB3	1:C:162:TYR:HA	2.00	0.42
1:D:165:ARG:O	1:D:221:GLY:HA3	2.19	0.42
1:D:285:TYR:CE1	1:D:411:ILE:HD12	2.54	0.42
1:G:367:TYR:CE2	1:G:398:GLY:HA2	2.53	0.42
1:B:367:TYR:HB3	2:B:420:SO4:O1	2.18	0.42
1:E:306:ASP:O	1:E:309:GLU:HG2	2.19	0.42
1:A:234:VAL:HG21	1:A:245:ILE:HG23	2.00	0.42
1:H:185:ARG:NH1	1:H:188:GLU:OE1	2.52	0.42
1:A:13:ILE:HG22	1:A:358:THR:HG21	2.00	0.42
1:B:29:GLU:O	1:C:347:ARG:HD3	2.19	0.42
1:A:160:ASN:C	3:A:422:PGE:H6	2.40	0.42
1:A:356:THR:HG22	5:A:2058:HOH:O	2.20	0.42
1:B:388:HIS:HA	2:B:420:SO4:O4	2.20	0.42
1:F:38:ARG:C	1:F:40:LEU:H	2.23	0.42
1:F:44:ILE:O	4:F:422:PG4:O2	2.38	0.42
1:H:249:LEU:HD11	1:H:262:VAL:HG11	2.01	0.42
1:D:160:ASN:ND2	5:D:2011:HOH:O	2.53	0.41
1:H:31:LEU:HD21	1:H:159:PRO:HG3	2.01	0.41
1:C:367:TYR:CE1	1:C:389:GLY:HA3	2.55	0.41
1:E:7:ILE:O	1:E:173:THR:HA	2.20	0.41
1:E:242:ALA:HA	1:E:245:ILE:HD12	2.02	0.41
1:C:31:LEU:HD21	1:C:159:PRO:HG3	2.02	0.41
1:A:369:ARG:HD2	2:A:420:SO4:O3	2.21	0.41
1:A:376:ILE:HG13	1:F:379:SER:HB2	2.01	0.41
1:F:47:LEU:HB3	4:F:422:PG4:H71	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:LYS:HG2	1:H:67:GLU:HB3	2.03	0.41
1:D:31:LEU:HD21	1:D:159:PRO:HG3	2.02	0.41
4:F:422:PG4:H11	1:G:351:ASN:OD1	2.21	0.41
1:A:35:TYR:HB3	1:A:38:ARG:HG2	2.03	0.40
1:D:217:THR:HG21	1:D:243:ALA:HB3	2.03	0.40
1:H:160:ASN:ND2	5:H:2006:HOH:O	2.50	0.40
1:A:338:GLY:HA3	1:A:345:ALA:HA	2.03	0.40
1:B:305:TYR:CE2	1:B:308:GLU:HA	2.56	0.40
1:D:285:TYR:HE1	1:D:411:ILE:HD12	1.85	0.40
1:G:252:ILE:HG23	1:G:257:LEU:HB2	2.04	0.40
1:H:405:PRO:HG2	1:H:408:ARG:NH1	2.36	0.40
1:C:338:GLY:HA3	1:C:345:ALA:HA	2.03	0.40
1:E:31:LEU:HD21	1:E:159:PRO:HG3	2.04	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	406/411 (99%)	389 (96%)	17 (4%)	0	100	100
1	B	409/411 (100%)	396 (97%)	12 (3%)	1 (0%)	47	66
1	C	407/411 (99%)	395 (97%)	12 (3%)	0	100	100
1	D	407/411 (99%)	396 (97%)	11 (3%)	0	100	100
1	E	404/411 (98%)	387 (96%)	17 (4%)	0	100	100
1	F	407/411 (99%)	386 (95%)	20 (5%)	1 (0%)	47	66
1	G	406/411 (99%)	394 (97%)	12 (3%)	0	100	100
1	H	406/411 (99%)	395 (97%)	11 (3%)	0	100	100
All	All	3252/3288 (99%)	3138 (96%)	112 (3%)	2 (0%)	51	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	307	ASN
1	F	39	LEU

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	352/354 (99%)	343 (97%)	9 (3%)	46	70
1	B	354/354 (100%)	344 (97%)	10 (3%)	43	67
1	C	352/354 (99%)	345 (98%)	7 (2%)	55	77
1	D	352/354 (99%)	342 (97%)	10 (3%)	43	67
1	E	350/354 (99%)	336 (96%)	14 (4%)	31	53
1	F	352/354 (99%)	341 (97%)	11 (3%)	40	64
1	G	352/354 (99%)	344 (98%)	8 (2%)	50	74
1	H	352/354 (99%)	341 (97%)	11 (3%)	40	64
All	All	2816/2832 (99%)	2736 (97%)	80 (3%)	43	67

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	37	GLU
1	A	40	LEU
1	A	41	PHE
1	A	218	ARG
1	A	255	GLN
1	A	352	ASP
1	A	396	ARG
1	A	401	CYS
1	B	1	MET
1	B	37	GLU
1	B	38	ARG

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Mol	Chain	Res	Type
1	B	42	ASP
1	B	150	ASN
1	B	185	ARG
1	B	330	GLU
1	B	337	CYS
1	B	352	ASP
1	B	396	ARG
1	C	36	LEU
1	C	42	ASP
1	C	183	GLU
1	C	212	ASP
1	C	271	ARG
1	C	310	LEU
1	C	347	ARG
1	D	37	GLU
1	D	42	ASP
1	D	115	GLU
1	D	212	ASP
1	D	249	LEU
1	D	261	LYS
1	D	271	ARG
1	D	297	ASP
1	D	396	ARG
1	D	401	CYS
1	E	8	HIS
1	E	37	GLU
1	E	73	THR
1	E	109	GLU
1	E	115	GLU
1	E	185	ARG
1	E	229	LYS
1	E	256	ASN
1	E	270	ASN
1	E	304	THR
1	E	307	ASN
1	E	336	ARG
1	E	337	CYS
1	E	396	ARG
1	F	38	ARG
1	F	40	LEU
1	F	41	PHE
1	F	115	GLU

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Mol	Chain	Res	Type
1	F	185	ARG
1	F	212	ASP
1	F	270	ASN
1	F	297	ASP
1	F	352	ASP
1	F	396	ARG
1	F	401	CYS
1	G	42	ASP
1	G	72	GLU
1	G	140	GLU
1	G	141	LYS
1	G	183	GLU
1	G	185	ARG
1	G	330	GLU
1	G	401	CYS
1	H	36	LEU
1	H	38	ARG
1	H	72	GLU
1	H	185	ARG
1	H	212	ASP
1	H	249	LEU
1	H	255	GLN
1	H	336	ARG
1	H	382	LEU
1	H	396	ARG
1	H	401	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	A	349	GLN
1	C	179	HIS
1	C	186	ASN
1	C	270	ASN
1	C	341	ASN
1	C	349	GLN
1	D	160	ASN
1	D	291	HIS
1	D	370	ASN
1	E	199	HIS
1	E	238	GLN

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Mol	Chain	Res	Type
1	F	97	ASN
1	F	160	ASN
1	F	355	ASN
1	F	388	HIS
1	G	186	ASN
1	G	214	ASN
1	G	326	ASN
1	G	349	GLN
1	G	355	ASN
1	H	351	ASN
1	H	388	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

19 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	F	420	-	4,4,4	0.82	0	6,6,6	0.76	0
2	SO4	E	420	-	4,4,4	0.39	0	6,6,6	0.22	0
2	SO4	B	420	-	4,4,4	0.63	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	420	-	4,4,4	0.73	0	6,6,6	0.51	0
2	SO4	B	421	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	D	421	-	4,4,4	0.25	0	6,6,6	0.15	0
2	SO4	H	420	-	4,4,4	0.84	0	6,6,6	0.37	0
2	SO4	G	420	-	4,4,4	0.59	0	6,6,6	0.42	0
4	PG4	F	422	-	12,12,12	0.28	0	11,11,11	0.36	0
2	SO4	F	421	-	4,4,4	0.25	0	6,6,6	0.36	0
2	SO4	H	421	-	4,4,4	0.09	0	6,6,6	0.23	0
2	SO4	E	421	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	G	421	-	4,4,4	0.25	0	6,6,6	0.30	0
3	PGE	A	422	-	9,9,9	0.40	0	8,8,8	0.41	0
2	SO4	A	421	-	4,4,4	0.16	0	6,6,6	0.37	0
3	PGE	F	423	-	9,9,9	0.39	0	8,8,8	0.40	0
2	SO4	C	421	-	4,4,4	0.13	0	6,6,6	0.25	0
2	SO4	D	420	-	4,4,4	0.69	0	6,6,6	0.59	0
2	SO4	C	420	-	4,4,4	0.94	0	6,6,6	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	F	423	-	-	6/7/7/7	-
4	PG4	F	422	-	-	6/10/10/10	-
3	PGE	A	422	-	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	422	PG4	O3-C5-C6-O4
3	F	423	PGE	O2-C3-C4-O3
4	F	422	PG4	O2-C3-C4-O3
3	F	423	PGE	C6-C5-O3-C4
4	F	422	PG4	O4-C7-C8-O5
3	A	422	PGE	C1-C2-O2-C3
3	A	422	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	F	422	PG4	C8-C7-O4-C6
3	F	423	PGE	C1-C2-O2-C3
4	F	422	PG4	O1-C1-C2-O2
3	A	422	PGE	O2-C3-C4-O3
4	F	422	PG4	C1-C2-O2-C3
3	A	422	PGE	C3-C4-O3-C5
3	F	423	PGE	C3-C4-O3-C5
3	F	423	PGE	C4-C3-O2-C2
3	F	423	PGE	O3-C5-C6-O4

There are no ring outliers.

12 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	420	SO4	4	0
2	E	420	SO4	3	0
2	B	420	SO4	3	0
2	A	420	SO4	2	0
2	H	420	SO4	1	0
2	G	420	SO4	3	0
4	F	422	PG4	14	0
3	A	422	PGE	20	0
3	F	423	PGE	4	0
2	C	421	SO4	1	0
2	D	420	SO4	2	0
2	C	420	SO4	3	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	408/411 (99%)	0.32	11 (2%) 54 56	21, 42, 79, 114	0
1	B	411/411 (100%)	0.45	19 (4%) 32 34	29, 59, 99, 119	0
1	C	409/411 (99%)	0.30	10 (2%) 59 61	25, 45, 76, 114	0
1	D	409/411 (99%)	0.35	11 (2%) 54 56	27, 48, 79, 107	0
1	E	406/411 (98%)	1.11	73 (17%) 1 1	35, 77, 118, 146	0
1	F	409/411 (99%)	0.32	10 (2%) 59 61	22, 43, 81, 111	0
1	G	408/411 (99%)	0.66	37 (9%) 9 8	27, 59, 101, 135	0
1	H	408/411 (99%)	0.90	55 (13%) 3 2	31, 65, 116, 159	0
All	All	3268/3288 (99%)	0.55	226 (6%) 16 16	21, 54, 103, 159	0

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	268	ALA	9.1
1	H	253	PHE	6.8
1	H	259	PHE	6.4
1	H	301	TYR	6.3
1	C	268	ALA	5.9
1	G	253	PHE	5.4
1	H	310	LEU	5.3
1	E	234	VAL	5.2
1	E	313	VAL	5.1
1	E	253	PHE	5.0
1	D	144	THR	4.9
1	E	273	PHE	4.7
1	H	267	PHE	4.6
1	H	266	GLU	4.5
1	B	253	PHE	4.4
1	H	250	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	225	LEU	4.3
1	E	260	LYS	4.3
1	B	144	THR	4.2
1	E	144	THR	4.2
1	H	327	LEU	4.2
1	E	269	ASN	4.2
1	E	340	ASP	4.2
1	B	143	LEU	4.0
1	A	42	ASP	4.0
1	H	260	LYS	3.9
1	H	311	HIS	3.9
1	F	253	PHE	3.9
1	G	307	ASN	3.9
1	G	305	TYR	3.9
1	B	294	ILE	3.9
1	E	140	GLU	3.8
1	G	310	LEU	3.8
1	E	262	VAL	3.8
1	C	269	ASN	3.8
1	H	249	LEU	3.8
1	H	305	TYR	3.8
1	G	259	PHE	3.7
1	E	250	VAL	3.7
1	H	306	ASP	3.7
1	C	144	THR	3.7
1	H	236	ILE	3.7
1	H	272	LYS	3.7
1	B	269	ASN	3.7
1	H	175	VAL	3.6
1	E	272	LYS	3.6
1	A	271	ARG	3.5
1	G	258	GLY	3.5
1	H	9	VAL	3.5
1	E	306	ASP	3.5
1	E	83	GLU	3.4
1	H	269	ASN	3.4
1	E	146	LEU	3.4
1	B	142	GLY	3.4
1	E	232	LEU	3.4
1	H	300	VAL	3.4
1	A	253	PHE	3.4
1	E	355	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	143	LEU	3.3
1	G	267	PHE	3.3
1	E	171	ILE	3.3
1	E	204	GLY	3.3
1	H	261	LYS	3.3
1	B	267	PHE	3.3
1	E	256	ASN	3.3
1	E	115	GLU	3.3
1	H	296	GLY	3.2
1	E	336	ARG	3.2
1	H	298	LEU	3.2
1	G	311	HIS	3.2
1	C	267	PHE	3.1
1	E	7	ILE	3.1
1	E	303	VAL	3.1
1	E	365	VAL	3.1
1	H	229	LYS	3.1
1	E	332	VAL	3.1
1	E	214	ASN	3.1
1	B	271	ARG	3.1
1	D	143	LEU	3.1
1	H	322	LEU	3.1
1	E	305	TYR	3.1
1	B	293	GLU	3.0
1	H	313	VAL	3.0
1	E	263	LEU	3.0
1	E	268	ALA	3.0
1	E	295	GLU	3.0
1	E	226	VAL	3.0
1	G	298	LEU	3.0
1	H	319	LEU	3.0
1	E	231	VAL	3.0
1	H	209	MET	3.0
1	E	142	GLY	3.0
1	E	136	ILE	2.9
1	E	259	PHE	2.9
1	H	263	LEU	2.9
1	H	307	ASN	2.9
1	G	210	VAL	2.9
1	E	323	LEU	2.9
1	E	114	ILE	2.9
1	H	411	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	231	VAL	2.9
1	G	233	ALA	2.9
1	G	249	LEU	2.9
1	E	329	VAL	2.9
1	H	299	ARG	2.9
1	G	272	LYS	2.9
1	G	262	VAL	2.9
1	G	236	ILE	2.8
1	A	273	PHE	2.8
1	D	4	GLN	2.8
1	H	302	SER	2.8
1	D	269	ASN	2.8
1	F	273	PHE	2.8
1	G	252	ILE	2.7
1	G	313	VAL	2.7
1	F	3	ALA	2.7
1	A	40	LEU	2.7
1	E	267	PHE	2.7
1	H	248	LEU	2.7
1	H	252	ILE	2.7
1	B	140	GLU	2.7
1	D	294	ILE	2.7
1	E	319	LEU	2.7
1	E	183	GLU	2.6
1	C	143	LEU	2.6
1	C	146	LEU	2.6
1	C	136	ILE	2.6
1	E	177	LEU	2.6
1	G	209	MET	2.6
1	G	297	ASP	2.6
1	D	136	ILE	2.6
1	E	252	ILE	2.6
1	E	294	ILE	2.6
1	E	359	ILE	2.6
1	G	301	TYR	2.6
1	E	210	VAL	2.5
1	B	225	LEU	2.5
1	H	210	VAL	2.5
1	E	216	THR	2.5
1	B	146	LEU	2.5
1	E	261	LYS	2.5
1	F	254	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	267	PHE	2.5
1	H	231	VAL	2.5
1	E	236	ILE	2.5
1	H	181	PHE	2.5
1	E	274	MET	2.5
1	E	175	VAL	2.4
1	F	136	ILE	2.4
1	F	294	ILE	2.4
1	E	292	PRO	2.4
1	G	269	ASN	2.4
1	H	273	PHE	2.4
1	H	144	THR	2.4
1	B	249	LEU	2.4
1	D	270	ASN	2.4
1	E	312	ILE	2.4
1	E	310	LEU	2.4
1	E	248	LEU	2.4
1	E	293	GLU	2.4
1	A	306	ASP	2.3
1	G	290	ILE	2.3
1	H	246	GLU	2.3
1	B	305	TYR	2.3
1	E	235	GLY	2.3
1	E	298	LEU	2.3
1	F	43	ASP	2.3
1	H	308	GLU	2.3
1	B	214	ASN	2.3
1	A	297	ASP	2.3
1	G	254	LYS	2.3
1	G	13	ILE	2.3
1	A	43	ASP	2.3
1	E	265	PHE	2.3
1	G	242	ALA	2.3
1	B	40	LEU	2.3
1	A	274	MET	2.3
1	D	411	ILE	2.3
1	E	86	GLU	2.3
1	G	312	ILE	2.2
1	G	411	ILE	2.2
1	E	79	LEU	2.2
1	H	146	LEU	2.2
1	H	171	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	101	ARG	2.2
1	H	303	VAL	2.2
1	A	268	ALA	2.2
1	G	181	PHE	2.2
1	F	39	LEU	2.2
1	B	340	ASP	2.2
1	G	296	GLY	2.2
1	G	306	ASP	2.2
1	H	204	GLY	2.2
1	H	256	ASN	2.2
1	H	316	LYS	2.2
1	E	102	ALA	2.2
1	D	273	PHE	2.2
1	G	177	LEU	2.2
1	E	215	GLU	2.2
1	G	175	VAL	2.2
1	H	214	ASN	2.2
1	E	109	GLU	2.2
1	E	337	CYS	2.2
1	E	275	HIS	2.1
1	C	273	PHE	2.1
1	E	194	TYR	2.1
1	H	251	ASN	2.1
1	H	295	GLU	2.1
1	G	9	VAL	2.1
1	G	7	ILE	2.1
1	F	37	GLU	2.1
1	H	242	ALA	2.1
1	C	184	THR	2.1
1	D	267	PHE	2.1
1	F	297	ASP	2.1
1	G	230	ASP	2.1
1	H	5	THR	2.1
1	H	276	LEU	2.1
1	B	257	LEU	2.0
1	C	137	PRO	2.0
1	H	228	SER	2.0
1	E	249	LEU	2.0
1	H	257	LEU	2.0
1	B	295	GLU	2.0
1	E	9	VAL	2.0
1	G	10	TYR	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. 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(\AA^2)	Q<0.9
4	PG4	F	422	13/13	0.82	0.29	59,62,67,68	0
2	SO4	H	421	5/5	0.82	0.35	94,95,96,96	5
3	PGE	F	423	10/10	0.82	0.29	49,60,66,67	0
3	PGE	A	422	10/10	0.87	0.37	35,41,43,44	0
2	SO4	D	421	5/5	0.88	0.28	79,80,80,80	5
2	SO4	E	421	5/5	0.89	0.16	101,101,102,102	5
2	SO4	B	421	5/5	0.92	0.19	91,91,91,91	5
2	SO4	D	420	5/5	0.92	0.36	26,30,34,36	5
2	SO4	C	420	5/5	0.93	0.28	21,26,30,34	5
2	SO4	G	421	5/5	0.94	0.19	52,54,57,58	5
2	SO4	E	420	5/5	0.95	0.43	34,37,39,43	5
2	SO4	G	420	5/5	0.96	0.31	25,26,33,35	5
2	SO4	C	421	5/5	0.96	0.21	57,58,60,60	5
2	SO4	B	420	5/5	0.96	0.41	30,30,34,37	5
2	SO4	A	420	5/5	0.96	0.31	16,19,20,24	5
2	SO4	H	420	5/5	0.97	0.24	26,29,36,37	5
2	SO4	F	421	5/5	0.97	0.16	55,56,57,62	0
2	SO4	A	421	5/5	0.98	0.15	46,51,52,54	0
2	SO4	F	420	5/5	0.99	0.21	18,20,22,23	5

6.5 Other polymers [i](#)

There are no such residues in this entry.