



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:27 PM UTC

PDB ID : 4BOF / pdb_00004bof
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 types of validation reports are described at

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

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

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

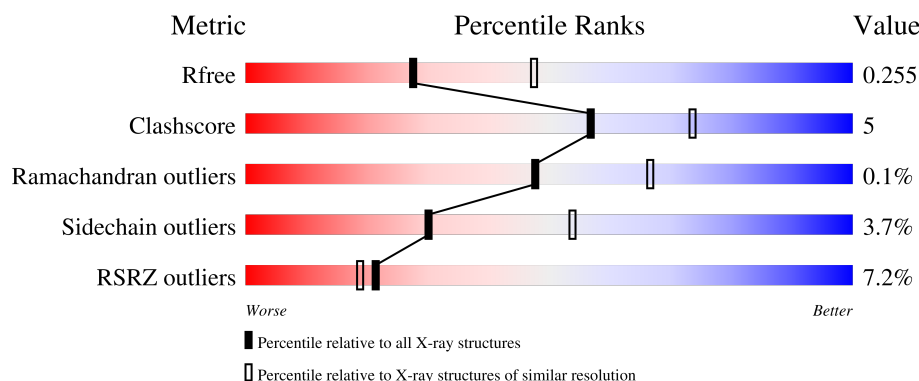
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	411	4% 84% 14% ..
1	B	411	6% 88% 11% .
1	C	411	5% 87% 11% .
1	D	411	3% 87% 12% .
1	E	411	20% 85% 14% .

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Mol	Chain	Length	Quality of chain
1	F	411	
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 (CCD ID: SO4) (formula: O₄S).



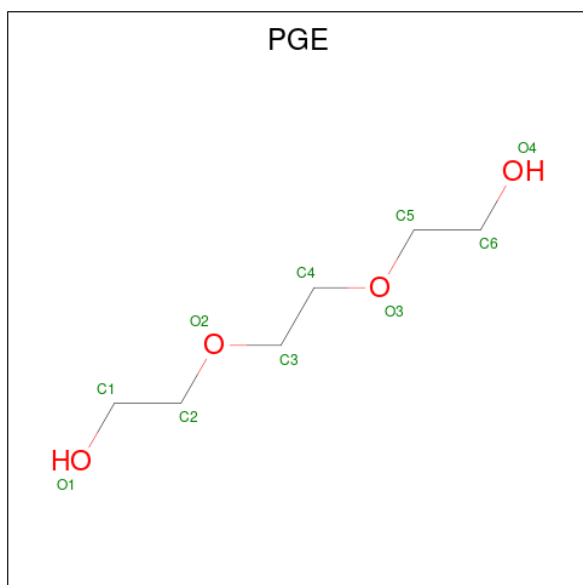
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	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 (CCD ID: 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 (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

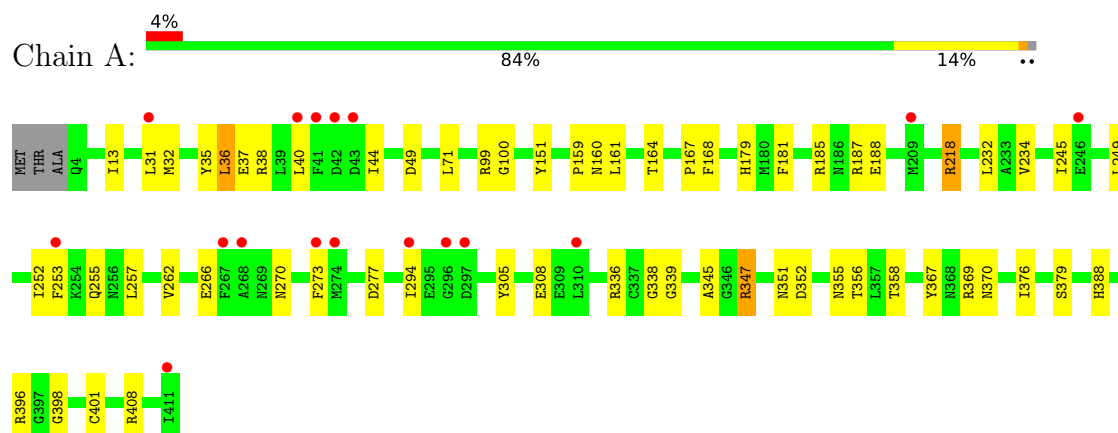
- Molecule 5 is water.

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		

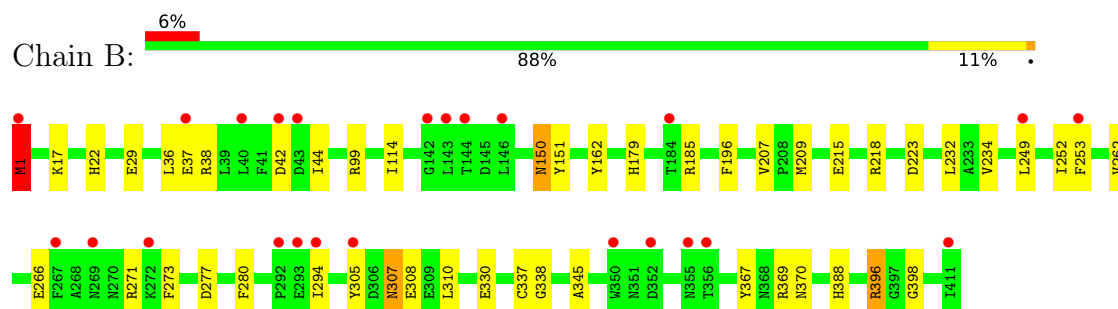
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

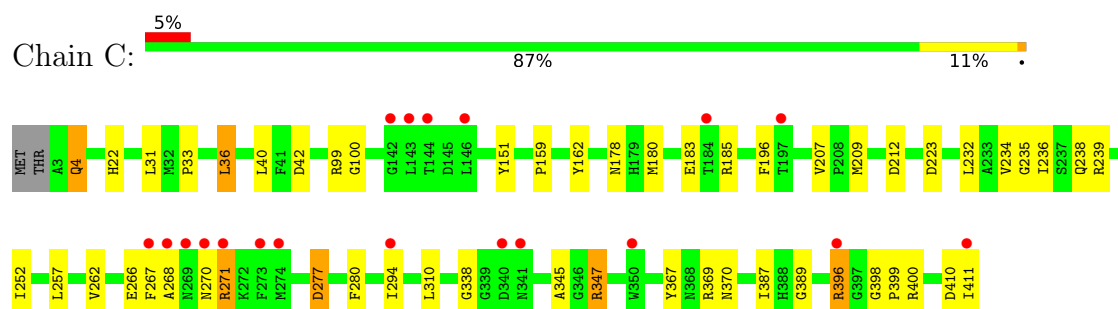
• Molecule 1: ARGININE DEIMINASE



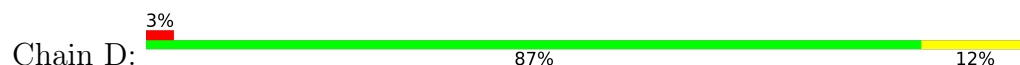
• Molecule 1: ARGININE DEIMINASE

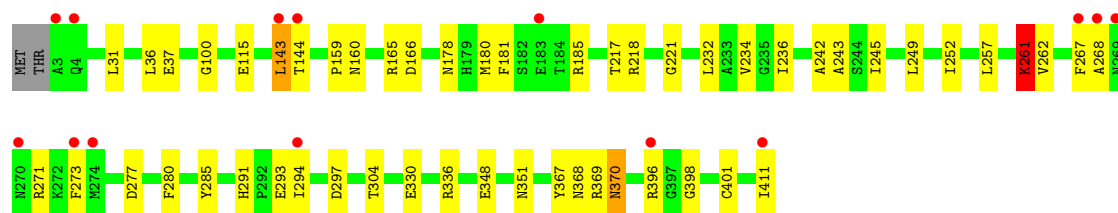


• Molecule 1: ARGININE DEIMINASE

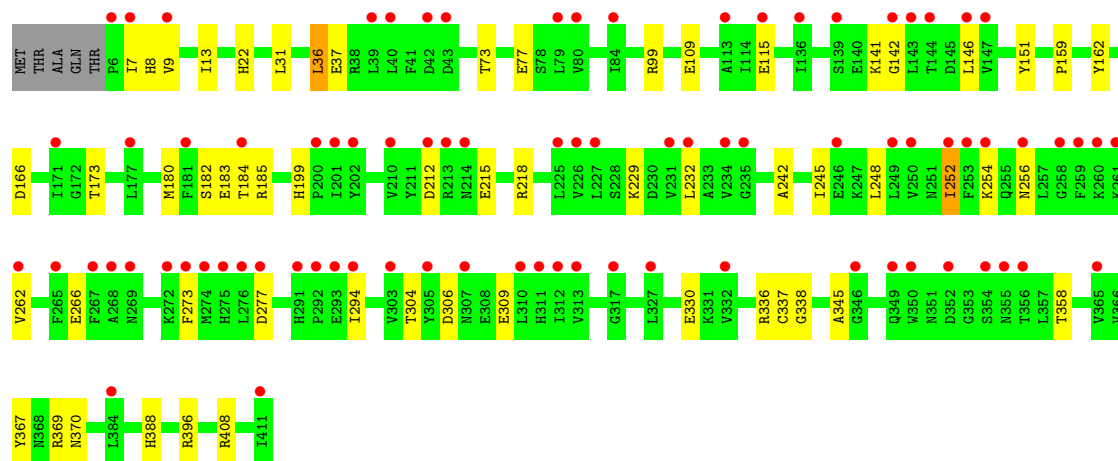
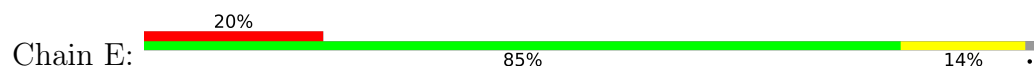


• Molecule 1: ARGININE DEIMINASE

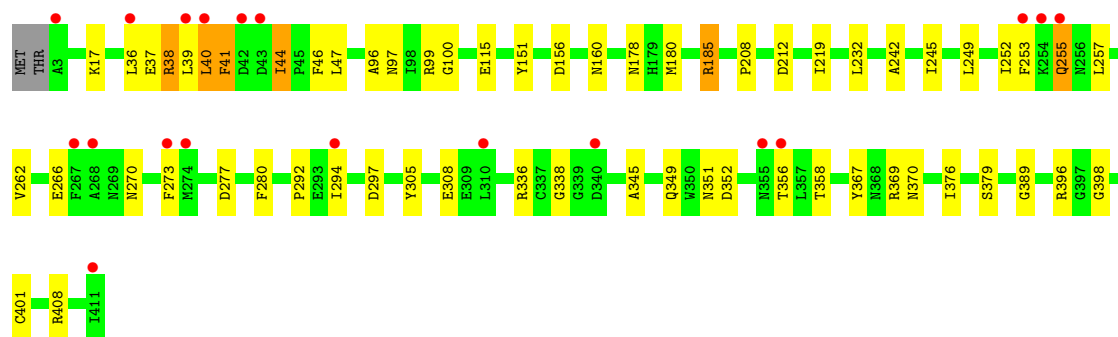
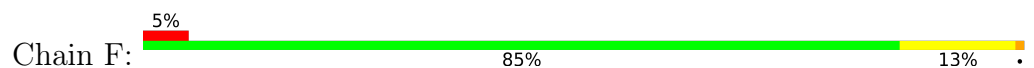




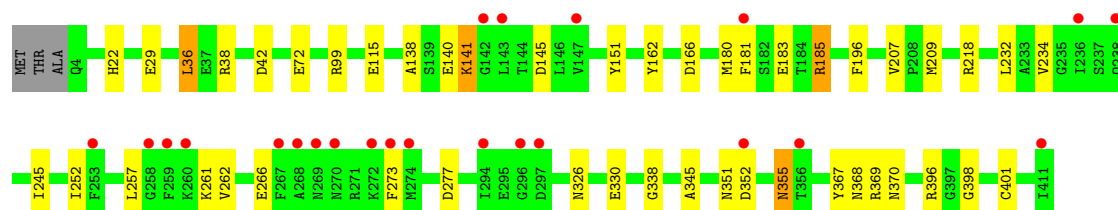
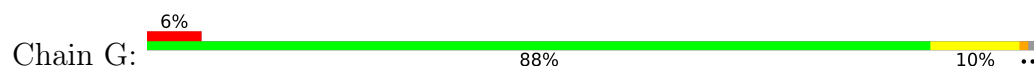
• Molecule 1: ARGININE DEIMINASE



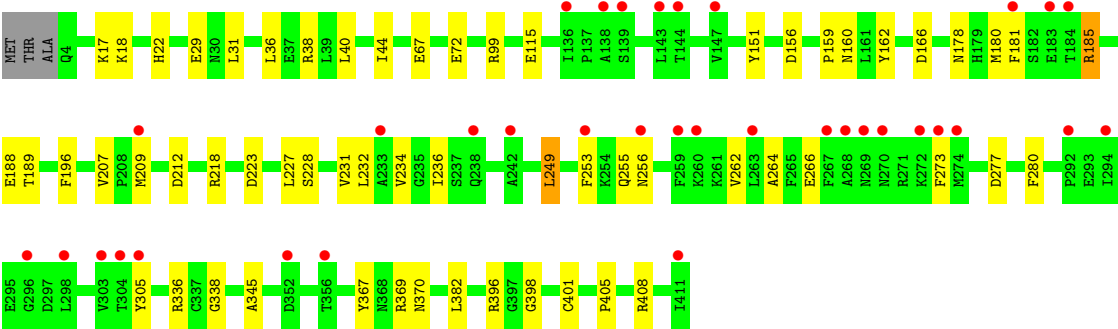
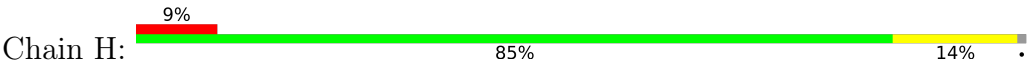
• Molecule 1: ARGININE DEIMINASE



• 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 36.31 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.31-2.48) 99.3 (36.31-2.48)	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 , 61.9	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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.91	1/3296 (0.0%)	1.32	18/4457 (0.4%)
1	B	0.83	1/3316 (0.0%)	1.29	16/4484 (0.4%)
1	C	0.88	0/3301	1.29	14/4464 (0.3%)
1	D	0.89	2/3301 (0.1%)	1.30	12/4464 (0.3%)
1	E	0.83	0/3280	1.29	9/4434 (0.2%)
1	F	0.90	0/3301	1.32	16/4464 (0.4%)
1	G	0.83	0/3296	1.27	7/4457 (0.2%)
1	H	0.82	0/3296	1.29	7/4457 (0.2%)
All	All	0.86	4/26387 (0.0%)	1.30	99/35681 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	SD-CE	-6.39	1.63	1.79
1	D	267	PHE	CA-C	5.33	1.59	1.53
1	D	261	LYS	CA-C	-5.14	1.46	1.52
1	A	44	ILE	CA-C	5.12	1.57	1.53

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	267	PHE	CA-C-N	8.87	131.97	120.44
1	D	267	PHE	C-N-CA	8.87	131.97	120.44
1	D	277	ASP	CA-CB-CG	8.77	121.37	112.60
1	C	277	ASP	CA-CB-CG	7.62	120.22	112.60
1	B	150	ASN	CA-CB-CG	7.31	119.91	112.60
1	G	277	ASP	CA-CB-CG	7.02	119.62	112.60
1	B	277	ASP	CA-CB-CG	6.82	119.42	112.60
1	H	277	ASP	CA-CB-CG	6.81	119.41	112.60
1	H	370	ASN	CA-C-N	6.75	129.65	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	370	ASN	C-N-CA	6.75	129.65	120.54
1	A	339	GLY	CA-C-N	6.71	129.26	120.28
1	A	339	GLY	C-N-CA	6.71	129.26	120.28
1	E	370	ASN	CA-C-N	6.61	129.46	120.54
1	E	370	ASN	C-N-CA	6.61	129.46	120.54
1	A	355	ASN	CA-CB-CG	6.60	119.20	112.60
1	E	277	ASP	CA-CB-CG	6.59	119.19	112.60
1	G	370	ASN	CA-C-N	6.40	129.18	120.54
1	G	370	ASN	C-N-CA	6.40	129.18	120.54
1	F	370	ASN	CA-C-N	6.39	129.17	120.54
1	F	370	ASN	C-N-CA	6.39	129.17	120.54
1	G	355	ASN	CA-CB-CG	6.38	118.98	112.60
1	F	41	PHE	CA-CB-CG	-6.34	107.46	113.80
1	C	410	ASP	CA-C-N	6.32	133.08	121.70
1	C	410	ASP	C-N-CA	6.32	133.08	121.70
1	A	277	ASP	CA-CB-CG	6.23	118.83	112.60
1	C	4	GLN	CA-C-N	6.04	135.52	123.56
1	C	4	GLN	C-N-CA	6.04	135.52	123.56
1	A	49	ASP	CA-C-N	6.01	128.33	120.28
1	A	49	ASP	C-N-CA	6.01	128.33	120.28
1	B	307	ASN	CA-C-N	5.99	130.63	122.07
1	B	307	ASN	C-N-CA	5.99	130.63	122.07
1	A	273	PHE	CA-C-N	5.97	128.20	120.44
1	A	273	PHE	C-N-CA	5.97	128.20	120.44
1	A	370	ASN	CA-C-N	5.95	128.57	120.54
1	A	370	ASN	C-N-CA	5.95	128.57	120.54
1	F	277	ASP	CA-CB-CG	5.91	118.51	112.60
1	D	370	ASN	CA-C-N	5.87	128.47	120.54
1	D	370	ASN	C-N-CA	5.87	128.47	120.54
1	F	273	PHE	CA-C-N	5.87	128.07	120.44
1	F	273	PHE	C-N-CA	5.87	128.07	120.44
1	E	273	PHE	CA-C-N	5.84	128.04	120.44
1	E	273	PHE	C-N-CA	5.84	128.04	120.44
1	B	370	ASN	CA-C-N	5.83	128.40	120.54
1	B	370	ASN	C-N-CA	5.83	128.40	120.54
1	F	351	ASN	CA-C-N	5.81	130.38	122.19
1	F	351	ASN	C-N-CA	5.81	130.38	122.19
1	H	256	ASN	CA-CB-CG	5.78	118.38	112.60
1	A	270	ASN	CA-C-N	5.77	130.35	120.72
1	A	270	ASN	C-N-CA	5.77	130.35	120.72
1	B	294	ILE	N-CA-C	5.77	116.55	110.72
1	E	212	ASP	CA-CB-CG	5.75	118.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	100	GLY	CA-C-N	5.63	128.10	120.38
1	F	100	GLY	C-N-CA	5.63	128.10	120.38
1	F	270	ASN	CA-C-N	5.63	132.33	121.18
1	F	270	ASN	C-N-CA	5.63	132.33	121.18
1	D	143	LEU	N-CA-C	5.61	117.09	110.97
1	C	370	ASN	CA-C-N	5.59	128.09	120.54
1	C	370	ASN	C-N-CA	5.59	128.09	120.54
1	F	349	GLN	CA-C-N	5.54	128.26	120.28
1	F	349	GLN	C-N-CA	5.54	128.26	120.28
1	E	215	GLU	CA-C-N	5.51	132.07	121.54
1	E	215	GLU	C-N-CA	5.51	132.07	121.54
1	A	351	ASN	CA-C-N	5.50	129.94	122.19
1	A	351	ASN	C-N-CA	5.50	129.94	122.19
1	A	187	ARG	CA-C-N	5.42	128.09	120.28
1	A	187	ARG	C-N-CA	5.42	128.09	120.28
1	E	36	LEU	N-CA-C	5.39	116.96	111.14
1	F	280	PHE	CA-CB-CG	5.38	119.18	113.80
1	G	273	PHE	CA-C-N	5.35	127.40	120.44
1	G	273	PHE	C-N-CA	5.35	127.40	120.44
1	G	36	LEU	N-CA-C	5.32	116.89	111.14
1	B	273	PHE	CA-C-N	5.25	127.27	120.44
1	B	273	PHE	C-N-CA	5.25	127.27	120.44
1	B	280	PHE	CA-CB-CG	5.25	119.05	113.80
1	C	178	ASN	N-CA-C	5.18	117.55	110.55
1	D	273	PHE	CA-C-N	5.17	127.16	120.44
1	D	273	PHE	C-N-CA	5.17	127.16	120.44
1	C	396	ARG	CB-CG-CD	5.16	123.17	111.30
1	H	273	PHE	CA-C-N	5.15	127.14	120.44
1	H	273	PHE	C-N-CA	5.15	127.14	120.44
1	C	235	GLY	CA-C-N	5.14	129.32	122.95
1	C	235	GLY	C-N-CA	5.14	129.32	122.95
1	C	280	PHE	CA-CB-CG	5.13	118.93	113.80
1	D	280	PHE	CA-CB-CG	5.13	118.93	113.80
1	F	44	ILE	O-C-N	-5.12	117.12	121.57
1	B	215	GLU	CA-C-N	5.12	127.09	120.44
1	B	215	GLU	C-N-CA	5.12	127.09	120.44
1	B	114	ILE	CA-C-N	5.09	127.36	120.44
1	B	114	ILE	C-N-CA	5.09	127.36	120.44
1	D	336	ARG	CA-C-N	5.07	128.05	120.95
1	D	336	ARG	C-N-CA	5.07	128.05	120.95
1	D	178	ASN	N-CA-C	5.07	117.39	110.55
1	C	271	ARG	CA-C-N	5.06	127.32	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	ARG	C-N-CA	5.06	127.32	120.38
1	B	271	ARG	CA-C-N	5.04	127.28	120.38
1	B	271	ARG	C-N-CA	5.04	127.28	120.38
1	H	280	PHE	CA-CB-CG	5.03	118.83	113.80
1	A	100	GLY	CA-C-N	5.01	126.99	120.28
1	A	100	GLY	C-N-CA	5.01	126.99	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3237	0	3231	48	0
1	B	3257	0	3255	22	0
1	C	3242	0	3236	27	0
1	D	3242	0	3236	24	0
1	E	3221	0	3217	24	0
1	F	3242	0	3236	42	0
1	G	3237	0	3231	28	0
1	H	3237	0	3231	30	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	238	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 5.

All (238) 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:H:196:PHE:HB3	1:H:209:MET:HE1	1.43	0.97
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:B:196:PHE:HB3	1:B:209:MET:HE1	1.47	0.95
1:G:369:ARG:HD2	2:G:420:SO4:O3	1.67	0.95
1:C:196:PHE:HB3	1:C:209:MET:HE1	1.49	0.94
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:G:196:PHE:HB3	1:G:209:MET:HE1	1.50	0.91
1:A:245:ILE:O	1:A:249:LEU:HG	1.75	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:166:ASP:HB3	1:G:180:MET:HE1	1.76	0.68
1:F:47:LEU:H	4:F:422:PG4:H62	1.58	0.67
1:B:1:MET:HE1	1:G:368:ASN:HB2	1.76	0.66
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:F:180:MET:HE2	1:F:185:ARG:NH1	2.12	0.64
1:G:207:VAL:O	1:G:209:MET:HE2	1.97	0.64
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:B:207:VAL:O	1:B:209:MET:HE2	1.97	0.63
1:A:358:THR:O	1:A:408:ARG:NH2	2.26	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:F:44:ILE:O	4:F:422:PG4:C1	2.47	0.61
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: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:H:180:MET:HE2	1:H:185:ARG:HG2	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: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:A:179:HIS:HD2	1:A:218:ARG:HG3	1.68	0.58
1:C:207:VAL:O	1:C:209:MET:HE2	2.03	0.58
1:D:234:VAL:HG21	1:D:245:ILE:HG12	1.85	0.58
1:A:347:ARG:HG2	1:H:44:ILE:HG21	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:180:MET:HE2	1:D:185:ARG:HB3	1.85	0.57
1:H:180:MET:CE	1:H:185:ARG:HG2	2.34	0.56
1:G:141:LYS:HG2	1:G:145:ASP:HB3	1.87	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:C:196:PHE:HB3	1:C:209:MET:CE	2.29	0.54
1:C:238:GLN:HG3	1:C:239:ARG:HG2	1.89	0.54
1:E:166:ASP:HB3	1:E:180:MET:HE1	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
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:C:180:MET:HE2	1:C:185:ARG:HB3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:LEU:HB2	1:C:262:VAL:HG22	1.93	0.51
1:B:196:PHE:HB3	1:B:209:MET:CE	2.32	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:H:207:VAL:O	1:H:209:MET:HE2	2.10	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:H:38:ARG:C	1:H:40:LEU:H	2.20	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:99:ARG:HH22	1:F:151:TYR:HB3	1.77	0.48
1:F:305:TYR:CE2	1:F:308:GLU:HA	2.48	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: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
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:A:160:ASN:C	3:A:422:PGE:H6	2.40	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:A:379:SER:HB2	1:F:376:ILE:CG1	2.45	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:F:38:ARG:C	1:F:40:LEU:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:MET:HE2	1:G:185:ARG:HG2	1.97	0.46
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:H:196:PHE:HB3	1:H:209:MET:CE	2.30	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:D:166:ASP:HB3	1:D:180:MET:HE1	1.98	0.45
1:F:208:PRO:HB3	1:F:255:GLN:HG2	1.98	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:SER:C	1:E:184:THR:H	2.25	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:G:196:PHE:HB3	1:G:209:MET:CE	2.35	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:H:166:ASP:HB3	1:H:180:MET:HE1	2.01	0.42
1:B:29:GLU:O	1:C:347:ARG:HD3	2.19	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: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:B:42:ASP:CG	1:B:396:ARG:HE	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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	406/411 (99%)	389 (96%)	17 (4%)	0	100	100
1	B	409/411 (100%)	396 (97%)	12 (3%)	1 (0%)	43	61
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%)	43	61
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%)	48	66

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%)	340 (97%)	12 (3%)	32	57
1	B	354/354 (100%)	342 (97%)	12 (3%)	32	57
1	C	352/354 (99%)	342 (97%)	10 (3%)	38	63
1	D	352/354 (99%)	340 (97%)	12 (3%)	32	57
1	E	350/354 (99%)	332 (95%)	18 (5%)	21	40
1	F	352/354 (99%)	337 (96%)	15 (4%)	26	48
1	G	352/354 (99%)	341 (97%)	11 (3%)	35	60
1	H	352/354 (99%)	338 (96%)	14 (4%)	28	51
All	All	2816/2832 (99%)	2712 (96%)	104 (4%)	30	54

All (104) 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	218	ARG
1	A	255	GLN
1	A	266	GLU
1	A	294	ILE
1	A	336	ARG
1	A	347	ARG
1	A	352	ASP
1	A	396	ARG
1	A	401	CYS
1	B	1	MET
1	B	17	LYS
1	B	36	LEU
1	B	37	GLU
1	B	38	ARG
1	B	150	ASN
1	B	185	ARG

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Mol	Chain	Res	Type
1	B	252	ILE
1	B	266	GLU
1	B	330	GLU
1	B	337	CYS
1	B	396	ARG
1	C	4	GLN
1	C	36	LEU
1	C	183	GLU
1	C	212	ASP
1	C	266	GLU
1	C	271	ARG
1	C	294	ILE
1	C	310	LEU
1	C	347	ARG
1	C	411	ILE
1	D	36	LEU
1	D	37	GLU
1	D	115	GLU
1	D	143	LEU
1	D	249	LEU
1	D	261	LYS
1	D	271	ARG
1	D	294	ILE
1	D	297	ASP
1	D	330	GLU
1	D	396	ARG
1	D	401	CYS
1	E	8	HIS
1	E	36	LEU
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	252	ILE
1	E	254	LYS
1	E	256	ASN
1	E	266	GLU
1	E	294	ILE
1	E	304	THR
1	E	330	GLU

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Mol	Chain	Res	Type
1	E	336	ARG
1	E	337	CYS
1	E	396	ARG
1	F	17	LYS
1	F	36	LEU
1	F	38	ARG
1	F	40	LEU
1	F	41	PHE
1	F	115	GLU
1	F	185	ARG
1	F	212	ASP
1	F	255	GLN
1	F	266	GLU
1	F	294	ILE
1	F	297	ASP
1	F	352	ASP
1	F	396	ARG
1	F	401	CYS
1	G	29	GLU
1	G	36	LEU
1	G	72	GLU
1	G	115	GLU
1	G	140	GLU
1	G	141	LYS
1	G	183	GLU
1	G	185	ARG
1	G	266	GLU
1	G	330	GLU
1	G	401	CYS
1	H	17	LYS
1	H	29	GLU
1	H	36	LEU
1	H	72	GLU
1	H	115	GLU
1	H	185	ARG
1	H	212	ASP
1	H	249	LEU
1	H	255	GLN
1	H	266	GLU
1	H	336	ARG
1	H	382	LEU
1	H	396	ARG

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Mol	Chain	Res	Type
1	H	401	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	A	368	ASN
1	B	307	ASN
1	B	349	GLN
1	B	368	ASN
1	C	179	HIS
1	C	186	ASN
1	C	270	ASN
1	C	349	GLN
1	C	368	ASN
1	D	8	HIS
1	D	129	GLN
1	D	160	ASN
1	D	179	HIS
1	D	291	HIS
1	D	349	GLN
1	D	368	ASN
1	D	370	ASN
1	E	199	HIS
1	E	238	GLN
1	E	270	ASN
1	E	368	ASN
1	F	97	ASN
1	F	160	ASN
1	F	256	ASN
1	F	349	GLN
1	F	355	ASN
1	F	368	ASN
1	F	388	HIS
1	G	186	ASN
1	G	251	ASN
1	G	326	ASN
1	G	349	GLN
1	H	214	ASN
1	H	388	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	421	-	4,4,4	0.22	0	6,6,6	0.17	0
2	SO4	G	421	-	4,4,4	0.26	0	6,6,6	0.29	0
2	SO4	H	421	-	4,4,4	0.17	0	6,6,6	0.24	0
2	SO4	A	421	-	4,4,4	0.27	0	6,6,6	0.38	0
2	SO4	E	420	-	4,4,4	0.36	0	6,6,6	0.21	0
2	SO4	C	421	-	4,4,4	0.18	0	6,6,6	0.26	0
2	SO4	C	420	-	4,4,4	0.91	0	6,6,6	0.72	0
2	SO4	G	420	-	4,4,4	0.61	0	6,6,6	0.41	0
2	SO4	E	421	-	4,4,4	0.26	0	6,6,6	0.15	0
2	SO4	A	420	-	4,4,4	0.59	0	6,6,6	0.51	0
2	SO4	H	420	-	4,4,4	0.76	0	6,6,6	0.34	0
4	PG4	F	422	-	12,12,12	0.28	0	11,11,11	0.36	0
2	SO4	D	421	-	4,4,4	0.34	0	6,6,6	0.18	0
3	PGE	F	423	-	9,9,9	0.39	0	8,8,8	0.39	0
2	SO4	D	420	-	4,4,4	0.55	0	6,6,6	0.58	0
3	PGE	A	422	-	9,9,9	0.40	0	8,8,8	0.40	0
2	SO4	F	420	-	4,4,4	0.69	0	6,6,6	0.74	0
2	SO4	F	421	-	4,4,4	0.30	0	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	420	-	4,4,4	0.51	0	6,6,6	0.25	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	A	422	-	-	4/7/7/7	-
3	PGE	F	423	-	-	6/7/7/7	-
4	PG4	F	422	-	-	6/10/10/10	-

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	A	422	PGE	C1-C2-O2-C3
3	F	423	PGE	C6-C5-O3-C4
3	F	423	PGE	C1-C2-O2-C3
4	F	422	PG4	C8-C7-O4-C6
4	F	422	PG4	O1-C1-C2-O2
4	F	422	PG4	O4-C7-C8-O5
3	A	422	PGE	C4-C3-O2-C2
4	F	422	PG4	C1-C2-O2-C3
3	A	422	PGE	O2-C3-C4-O3
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	E	420	SO4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	421	SO4	1	0
2	C	420	SO4	3	0
2	G	420	SO4	3	0
2	A	420	SO4	2	0
2	H	420	SO4	1	0
4	F	422	PG4	14	0
3	F	423	PGE	4	0
2	D	420	SO4	2	0
3	A	422	PGE	20	0
2	F	420	SO4	4	0
2	B	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	17 (4%)	40	36	21, 42, 79, 114	0
1	B	411/411 (100%)	0.56	24 (5%)	29	25	29, 59, 99, 119	0
1	C	409/411 (99%)	0.33	19 (4%)	37	33	25, 45, 76, 114	0
1	D	409/411 (99%)	0.44	14 (3%)	48	44	27, 48, 79, 107	0
1	E	406/411 (98%)	1.25	83 (20%)	3	2	34, 77, 118, 146	0
1	F	409/411 (99%)	0.40	19 (4%)	37	33	22, 43, 81, 111	0
1	G	408/411 (99%)	0.60	23 (5%)	30	26	27, 59, 101, 135	0
1	H	408/411 (99%)	0.77	35 (8%)	16	14	31, 65, 116, 159	0
All	All	3268/3288 (99%)	0.58	234 (7%)	21	19	21, 54, 103, 159	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	ASP	6.2
1	C	268	ALA	6.0
1	D	268	ALA	6.0
1	E	411	ILE	5.2
1	B	143	LEU	4.6
1	E	143	LEU	4.4
1	E	234	VAL	4.3
1	E	273	PHE	4.3
1	E	313	VAL	4.3
1	H	411	ILE	4.2
1	D	411	ILE	4.1
1	D	144	THR	4.1
1	C	267	PHE	4.1
1	B	411	ILE	4.0
1	A	273	PHE	3.8
1	G	267	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	411	ILE	3.7
1	D	3	ALA	3.7
1	F	273	PHE	3.6
1	H	267	PHE	3.6
1	F	294	ILE	3.6
1	H	272	LYS	3.6
1	A	43	ASP	3.6
1	F	43	ASP	3.6
1	E	144	THR	3.5
1	H	273	PHE	3.5
1	D	273	PHE	3.5
1	A	40	LEU	3.4
1	E	312	ILE	3.4
1	B	355	ASN	3.4
1	H	305	TYR	3.4
1	D	270	ASN	3.4
1	C	144	THR	3.4
1	E	253	PHE	3.3
1	C	396	ARG	3.3
1	A	411	ILE	3.3
1	G	273	PHE	3.2
1	E	310	LEU	3.2
1	C	273	PHE	3.2
1	B	142	GLY	3.2
1	E	43	ASP	3.2
1	H	269	ASN	3.2
1	E	227	LEU	3.2
1	D	267	PHE	3.1
1	B	267	PHE	3.1
1	H	253	PHE	3.1
1	E	250	VAL	3.1
1	E	274	MET	3.1
1	E	225	LEU	3.1
1	H	242	ALA	3.1
1	A	209	MET	3.1
1	A	274	MET	3.0
1	B	40	LEU	3.0
1	E	267	PHE	3.0
1	E	142	GLY	3.0
1	H	296	GLY	3.0
1	C	294	ILE	3.0
1	E	272	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	272	LYS	3.0
1	F	411	ILE	3.0
1	E	356	THR	3.0
1	B	43	ASP	3.0
1	F	253	PHE	3.0
1	H	268	ALA	2.9
1	F	254	LYS	2.9
1	D	183	GLU	2.9
1	F	274	MET	2.9
1	H	270	ASN	2.9
1	H	143	LEU	2.9
1	A	297	ASP	2.9
1	G	270	ASN	2.9
1	B	146	LEU	2.9
1	B	253	PHE	2.9
1	E	355	ASN	2.8
1	C	270	ASN	2.8
1	A	268	ALA	2.8
1	H	184	THR	2.8
1	E	260	LYS	2.8
1	B	294	ILE	2.8
1	E	177	LEU	2.8
1	F	42	ASP	2.8
1	E	252	ILE	2.7
1	E	6	PRO	2.7
1	F	355	ASN	2.7
1	C	146	LEU	2.7
1	G	143	LEU	2.7
1	E	352	ASP	2.7
1	F	40	LEU	2.7
1	B	292	PRO	2.7
1	A	267	PHE	2.7
1	G	253	PHE	2.7
1	A	294	ILE	2.6
1	B	144	THR	2.6
1	E	275	HIS	2.6
1	C	269	ASN	2.6
1	C	341	ASN	2.6
1	E	268	ALA	2.6
1	E	254	LYS	2.6
1	H	139	SER	2.6
1	E	292	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	147	VAL	2.6
1	G	269	ASN	2.6
1	B	305	TYR	2.6
1	H	274	MET	2.5
1	H	136	ILE	2.5
1	H	298	LEU	2.5
1	F	3	ALA	2.5
1	G	268	ALA	2.5
1	H	260	LYS	2.5
1	G	297	ASP	2.5
1	B	356	THR	2.5
1	C	184	THR	2.5
1	G	274	MET	2.5
1	E	305	TYR	2.5
1	D	294	ILE	2.5
1	E	171	ILE	2.5
1	E	293	GLU	2.5
1	C	143	LEU	2.5
1	E	147	VAL	2.5
1	E	262	VAL	2.5
1	C	271	ARG	2.5
1	E	139	SER	2.5
1	G	296	GLY	2.5
1	E	294	ILE	2.5
1	E	276	LEU	2.5
1	C	350	TRP	2.5
1	G	181	PHE	2.5
1	H	292	PRO	2.4
1	E	42	ASP	2.4
1	G	236	ILE	2.4
1	H	294	ILE	2.4
1	E	231	VAL	2.4
1	H	209	MET	2.4
1	B	352	ASP	2.4
1	H	238	GLN	2.4
1	H	259	PHE	2.4
1	D	274	MET	2.4
1	B	42	ASP	2.4
1	E	136	ILE	2.4
1	G	294	ILE	2.4
1	F	39	LEU	2.4
1	E	265	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	226	VAL	2.4
1	E	303	VAL	2.4
1	H	138	ALA	2.4
1	E	311	HIS	2.4
1	A	253	PHE	2.4
1	E	261	LYS	2.4
1	C	142	GLY	2.3
1	B	249	LEU	2.3
1	E	181	PHE	2.3
1	H	304	THR	2.3
1	A	296	GLY	2.3
1	E	213	ARG	2.3
1	G	259	PHE	2.3
1	H	183	GLU	2.3
1	F	268	ALA	2.3
1	E	349	GLN	2.3
1	G	258	GLY	2.3
1	H	263	LEU	2.3
1	G	260	LYS	2.3
1	E	115	GLU	2.3
1	E	113	ALA	2.3
1	C	411	ILE	2.3
1	E	232	LEU	2.3
1	E	327	LEU	2.3
1	F	310	LEU	2.3
1	H	144	THR	2.2
1	E	7	ILE	2.2
1	E	277	ASP	2.2
1	B	293	GLU	2.2
1	E	200	PRO	2.2
1	E	210	VAL	2.2
1	E	307	ASN	2.2
1	E	258	GLY	2.2
1	E	201	ILE	2.2
1	G	352	ASP	2.2
1	H	352	ASP	2.2
1	H	181	PHE	2.2
1	H	233	ALA	2.2
1	E	202	TYR	2.2
1	G	356	THR	2.2
1	H	356	THR	2.2
1	D	143	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	79	LEU	2.2
1	E	235	GLY	2.2
1	E	384	LEU	2.2
1	G	142	GLY	2.2
1	B	269	ASN	2.2
1	E	214	ASN	2.2
1	G	238	GLN	2.2
1	F	36	LEU	2.2
1	E	246	GLU	2.2
1	E	350	TRP	2.2
1	E	259	PHE	2.2
1	E	365	VAL	2.1
1	E	256	ASN	2.1
1	C	340	ASP	2.1
1	E	80	VAL	2.1
1	H	303	VAL	2.1
1	E	269	ASN	2.1
1	E	39	LEU	2.1
1	E	249	LEU	2.1
1	E	317	GLY	2.1
1	E	354	SER	2.1
1	E	332	VAL	2.1
1	H	147	VAL	2.1
1	F	356	THR	2.1
1	B	37	GLU	2.1
1	A	41	PHE	2.1
1	E	9	VAL	2.1
1	F	267	PHE	2.1
1	E	346	GLY	2.1
1	C	197	THR	2.1
1	E	184	THR	2.1
1	B	1	MET	2.1
1	A	310	LEU	2.0
1	E	40	LEU	2.0
1	B	184	THR	2.0
1	B	350	TRP	2.0
1	E	84	ILE	2.0
1	E	212	ASP	2.0
1	F	340	ASP	2.0
1	C	274	MET	2.0
1	D	4	GLN	2.0
1	F	255	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	396	ARG	2.0
1	A	31	LEU	2.0
1	A	246	GLU	2.0
1	E	146	LEU	2.0
1	B	272	LYS	2.0
1	D	269	ASN	2.0
1	H	256	ASN	2.0
1	E	291	HIS	2.0

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PGE	F	423	10/10	0.75	0.19	49,60,66,67	0
2	SO4	H	421	5/5	0.77	0.18	94,95,96,96	5
4	PG4	F	422	13/13	0.78	0.18	59,62,67,68	0
2	SO4	E	421	5/5	0.85	0.12	101,101,102,102	5
3	PGE	A	422	10/10	0.85	0.24	35,41,43,44	0
2	SO4	D	421	5/5	0.86	0.16	79,80,80,80	5
2	SO4	B	421	5/5	0.87	0.12	91,91,91,91	5
2	SO4	C	421	5/5	0.90	0.11	57,58,60,60	5
2	SO4	G	421	5/5	0.90	0.12	52,54,57,58	5
2	SO4	B	420	5/5	0.91	0.21	30,30,34,37	5
2	SO4	E	420	5/5	0.91	0.18	34,37,39,43	5
2	SO4	C	420	5/5	0.92	0.16	21,26,30,34	5
2	SO4	G	420	5/5	0.93	0.18	25,26,33,35	5
2	SO4	A	420	5/5	0.94	0.17	16,19,20,24	5
2	SO4	H	420	5/5	0.94	0.18	26,29,36,37	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	420	5/5	0.94	0.18	26,30,34,36	5
2	SO4	F	421	5/5	0.96	0.10	55,56,57,62	0
2	SO4	A	421	5/5	0.97	0.12	46,51,52,54	0
2	SO4	F	420	5/5	0.97	0.13	18,20,22,23	5

6.5 Other polymers [i](#)

There are no such residues in this entry.