



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:42 AM UTC

PDB ID : 3IR1 / pdb_00003ir1
Title : Crystal Structure of Lipoprotein GNA1946 from Neisseria meningitidis
Authors : Yang, X.; Wu, Z.; Wang, X.; Shen, Y.
Deposited on : 2009-08-21
Resolution : 2.15 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:

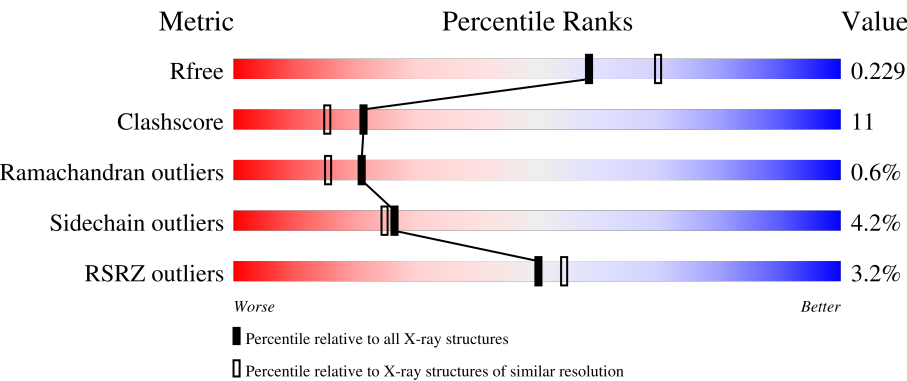
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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.



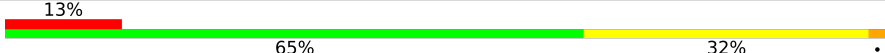
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	245	75%20%..
1	B	245	2% 73%23%.
1	C	245	2% 72%22%..
1	D	245	2% 73%22%..
1	E	245	77%18%..

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Mol	Chain	Length	Quality of chain
1	F	245	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	F	1	-	-	X	-

2 Entry composition [i](#)

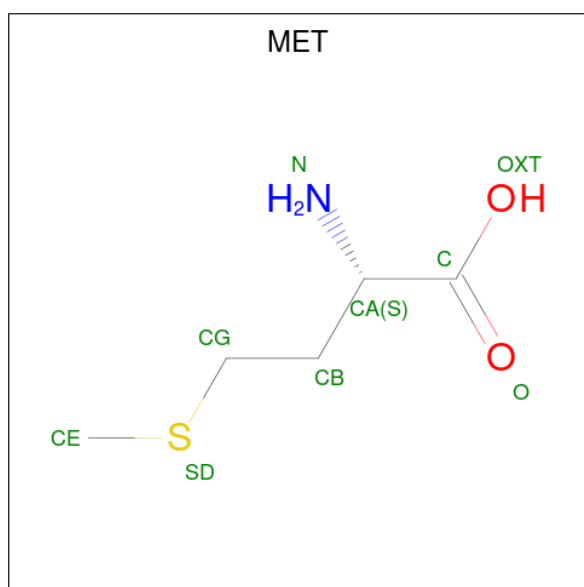
There are 4 unique types of molecules in this entry. The entry contains 12231 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Outer membrane lipoprotein GNA1946.

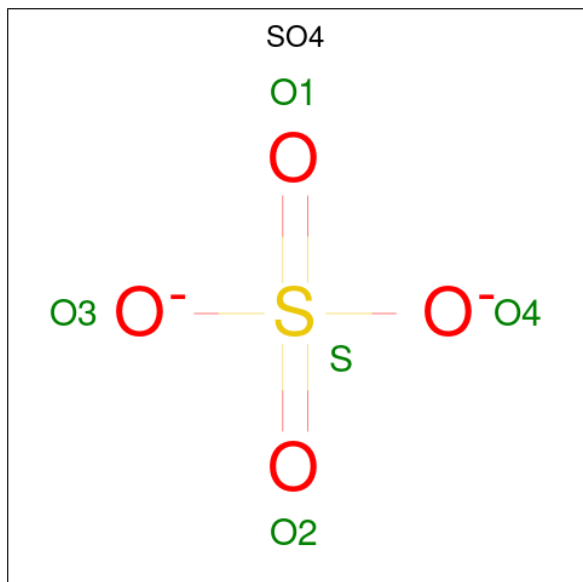
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1884	1211	305	365	3			
1	B	244	Total	C	N	O	S	0	0	0
			1919	1231	312	373	3			
1	C	239	Total	C	N	O	S	0	0	0
			1884	1211	305	365	3			
1	D	239	Total	C	N	O	S	0	0	0
			1884	1211	305	365	3			
1	E	239	Total	C	N	O	S	0	0	0
			1884	1211	305	365	3			
1	F	244	Total	C	N	O	S	0	0	0
			1915	1228	311	373	3			

- Molecule 2 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	C	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	D	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	E	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	F	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

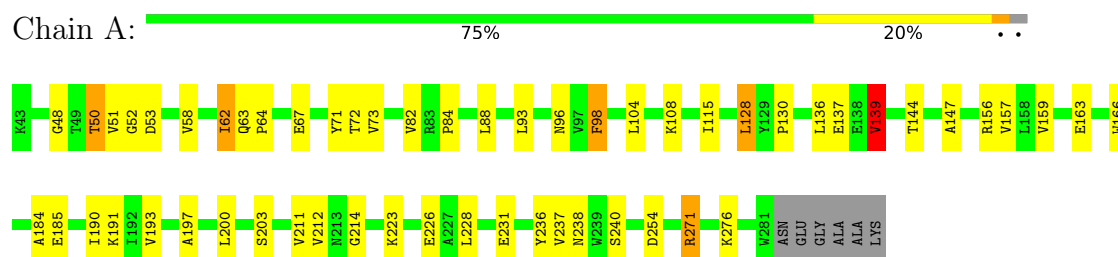
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	117	Total	O	0	0
			117	117		
4	C	117	Total	O	0	0
			117	117		
4	D	127	Total	O	0	0
			127	127		
4	E	127	Total	O	0	0
			127	127		
4	F	107	Total	O	0	0
			107	107		

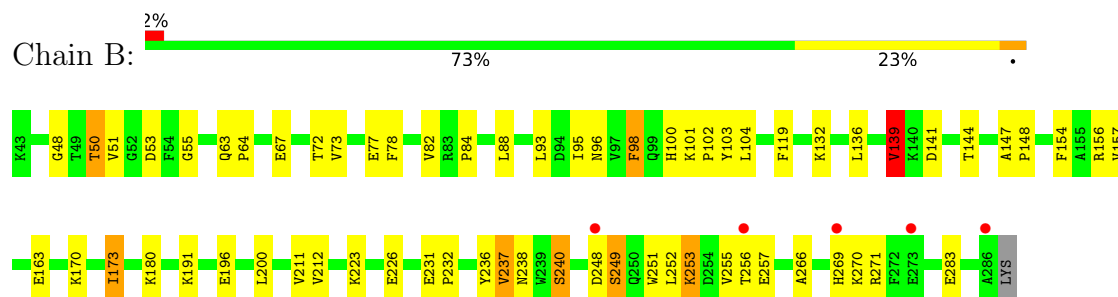
3 Residue-property plots [i](#)

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.

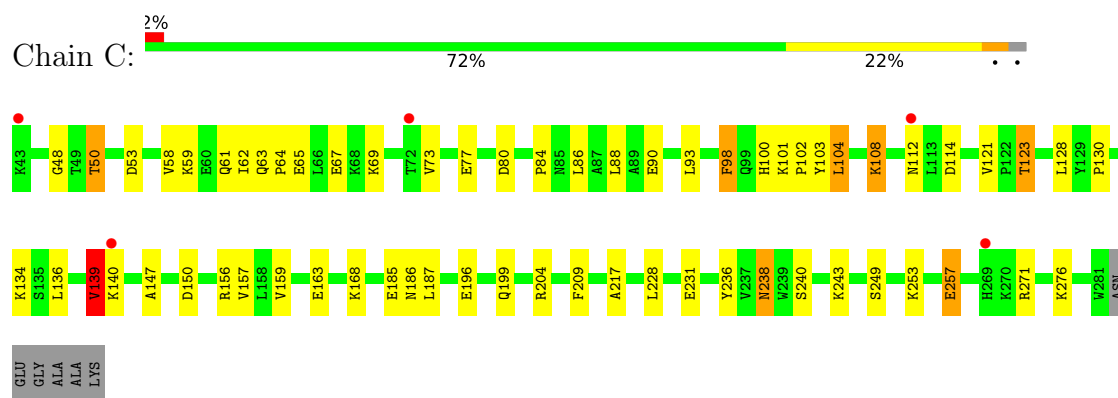
• Molecule 1: Outer membrane lipoprotein GNA1946



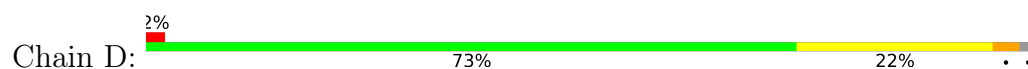
• Molecule 1: Outer membrane lipoprotein GNA1946

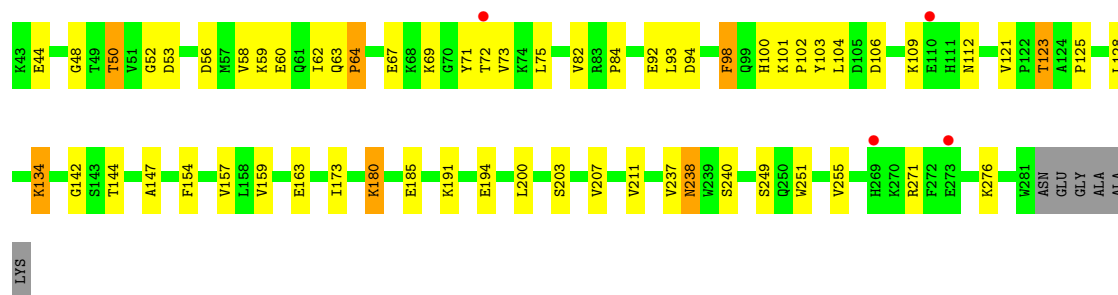


• Molecule 1: Outer membrane lipoprotein GNA1946



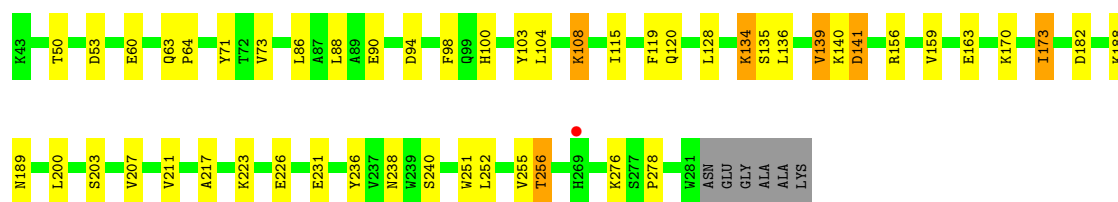
• Molecule 1: Outer membrane lipoprotein GNA1946





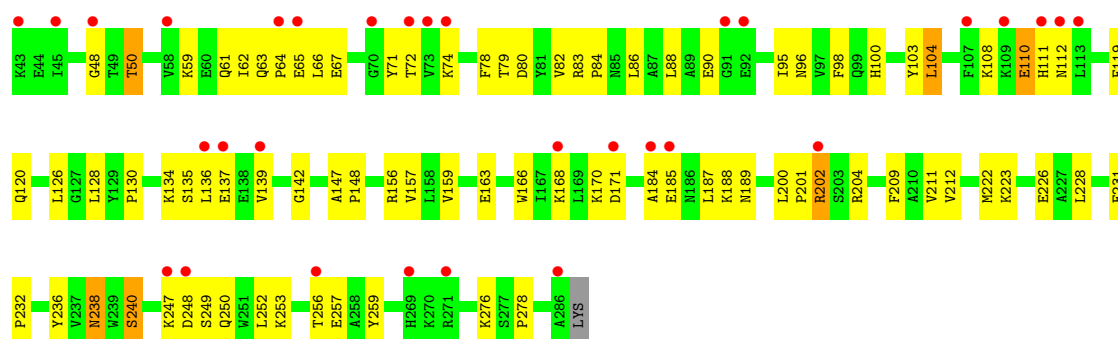
- Molecule 1: Outer membrane lipoprotein GNA1946

Chain E: 77% 18%



- Molecule 1: Outer membrane lipoprotein GNA1946

Chain F: 13% 65% 32%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.22Å 122.75Å 160.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.06 – 2.15 29.06 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.1 (29.06-2.15) 92.2 (29.06-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 2.16Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.204 , 0.229 0.204 , 0.229	Depositor DCC
R_{free} test set	5658 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12231	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: 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	0.43	0/1927	0.98	11/2615 (0.4%)
1	B	0.41	0/1962	0.98	10/2661 (0.4%)
1	C	0.40	0/1927	0.95	16/2615 (0.6%)
1	D	0.41	0/1927	0.97	9/2615 (0.3%)
1	E	0.42	0/1927	0.94	8/2615 (0.3%)
1	F	0.39	0/1958	0.97	7/2657 (0.3%)
All	All	0.41	0/11628	0.97	61/15778 (0.4%)

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	82	VAL	N-CA-C	9.42	119.96	110.82
1	A	139	VAL	CB-CA-C	-8.28	100.62	111.13
1	D	53	ASP	N-CA-C	8.21	120.97	111.11
1	A	82	VAL	N-CA-C	7.53	119.21	111.00
1	B	82	VAL	N-CA-C	7.46	118.06	110.82
1	D	52	GLY	N-CA-C	7.30	120.43	111.45
1	C	134	LYS	N-CA-C	6.82	121.76	113.17
1	E	53	ASP	N-CA-C	6.80	119.27	111.11
1	B	240	SER	N-CA-C	-6.79	100.47	110.52
1	B	53	ASP	N-CA-C	6.68	119.13	111.11
1	A	50	THR	N-CA-C	-6.64	100.65	110.48
1	B	212	VAL	N-CA-C	6.56	117.36	108.17
1	A	53	ASP	N-CA-C	6.51	118.93	111.11
1	E	50	THR	N-CA-C	-6.42	101.88	110.55
1	C	50	THR	N-CA-C	-6.36	101.97	110.55
1	F	240	SER	N-CA-C	-6.23	101.30	110.52
1	C	139	VAL	CB-CA-C	-6.12	102.08	111.08
1	D	82	VAL	N-CA-C	6.04	117.98	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	170	LYS	N-CA-C	-6.03	101.48	110.23
1	B	237	VAL	N-CA-C	-5.99	101.82	109.30
1	D	109	LYS	N-CA-C	-5.87	104.24	111.40
1	C	53	ASP	N-CA-C	5.80	118.07	111.11
1	A	72	THR	N-CA-C	-5.80	99.73	109.07
1	E	240	SER	N-CA-C	-5.74	102.80	110.55
1	B	72	THR	N-CA-C	-5.74	100.35	109.59
1	B	50	THR	N-CA-C	-5.74	102.81	110.55
1	D	50	THR	N-CA-C	-5.74	103.13	110.53
1	E	134	LYS	N-CA-C	5.74	120.34	113.23
1	A	240	SER	N-CA-C	-5.73	101.20	110.32
1	A	237	VAL	N-CA-C	-5.67	101.72	109.37
1	E	217	ALA	N-CA-C	-5.63	105.15	111.28
1	A	203	SER	N-CA-C	-5.58	105.97	112.89
1	F	59	LYS	N-CA-C	5.58	117.44	111.36
1	D	240	SER	N-CA-C	-5.56	103.04	110.55
1	F	238	ASN	N-CA-C	5.51	118.27	110.50
1	E	94	ASP	N-CA-C	-5.50	106.70	113.41
1	C	187	LEU	N-CA-C	5.48	117.96	111.33
1	C	217	ALA	N-CA-C	-5.44	105.25	111.07
1	D	238	ASN	N-CA-C	5.42	118.14	110.50
1	A	212	VAL	N-CA-C	5.38	116.34	108.53
1	C	73	VAL	N-CA-C	5.37	115.63	108.11
1	B	196	GLU	N-CA-C	-5.37	102.34	110.28
1	C	240	SER	N-CA-C	-5.35	102.61	110.52
1	F	50	THR	N-CA-C	-5.33	103.00	110.35
1	F	212	VAL	N-CA-C	5.30	115.53	108.11
1	C	150	ASP	CA-C-N	5.29	124.74	119.24
1	C	150	ASP	C-N-CA	5.29	124.74	119.24
1	C	196	GLU	N-CA-C	-5.28	102.46	110.28
1	B	139	VAL	CB-CA-C	-5.25	102.68	111.29
1	C	243	LYS	N-CA-C	-5.25	102.51	110.28
1	D	94	ASP	N-CA-C	-5.23	107.03	113.41
1	E	141	ASP	N-CA-C	-5.19	102.18	109.96
1	A	214	GLY	N-CA-C	5.18	118.94	112.73
1	C	238	ASN	N-CA-C	5.18	117.80	110.50
1	B	141	ASP	N-CA-C	-5.16	102.22	109.96
1	C	204	ARG	N-CA-C	5.14	118.66	112.38
1	E	60	GLU	N-CA-C	5.08	118.63	112.23
1	C	80	ASP	N-CA-C	5.06	117.95	109.96
1	D	73	VAL	N-CA-C	5.05	115.86	108.53
1	C	186	ASN	N-CA-C	-5.02	102.63	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ILE	N-CA-C	5.01	115.23	110.42

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	1884	0	1855	33	0
1	B	1919	0	1891	48	0
1	C	1884	0	1855	42	0
1	D	1884	0	1855	37	0
1	E	1884	0	1855	30	0
1	F	1915	0	1880	60	0
2	A	9	0	8	0	0
2	B	9	0	8	2	0
2	C	9	0	8	1	0
2	D	9	0	8	0	0
2	E	9	0	8	1	0
2	F	9	0	8	1	0
3	A	10	0	0	1	0
3	B	15	0	0	1	0
3	C	25	0	0	2	0
3	D	15	0	0	2	0
3	E	20	0	0	2	0
3	F	5	0	0	2	0
4	A	122	0	0	0	0
4	B	117	0	0	4	0
4	C	117	0	0	2	0
4	D	127	0	0	2	0
4	E	127	0	0	1	0
4	F	107	0	0	6	0
All	All	12231	0	11239	248	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 (248) 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:C:123:THR:HG21	1:C:238:ASN:H	1.06	1.20
1:D:123:THR:HG21	1:D:238:ASN:H	1.08	1.14
1:C:123:THR:HG21	1:C:238:ASN:N	1.90	0.85
1:D:123:THR:HG21	1:D:238:ASN:N	1.91	0.83
1:F:139:VAL:HG21	1:F:166:TRP:CZ2	2.14	0.82
1:B:63:GLN:HG3	1:B:73:VAL:HB	1.63	0.80
1:F:156:ARG:HD2	1:F:231:GLU:OE2	1.84	0.76
1:A:63:GLN:HG3	1:A:73:VAL:HB	1.67	0.75
1:C:130:PRO:HG3	1:C:228:LEU:HD21	1.69	0.75
1:C:140:LYS:HE3	4:C:845:HOH:O	1.87	0.75
1:B:252:LEU:O	1:B:256:THR:HG23	1.87	0.74
1:E:63:GLN:HG3	1:E:73:VAL:HB	1.70	0.73
1:F:104:LEU:CD2	1:F:108:LYS:HD3	2.19	0.73
1:B:136:LEU:O	1:B:139:VAL:HG22	1.90	0.71
1:B:156:ARG:HD2	1:B:231:GLU:OE2	1.89	0.71
1:D:44:GLU:HG3	1:D:72:THR:HG23	1.72	0.71
1:F:80:ASP:OD2	1:F:83:ARG:HG2	1.90	0.71
1:D:125:PRO:HB3	1:D:276:LYS:HE2	1.71	0.70
1:A:166:TRP:HB3	1:A:190:ILE:CD1	2.21	0.70
1:B:63:GLN:HB3	1:B:64:PRO:HD3	1.72	0.70
1:E:170:LYS:O	1:E:173:ILE:HD12	1.91	0.69
1:F:247:LYS:O	1:F:252:LEU:HD23	1.93	0.69
1:F:159:VAL:O	1:F:163:GLU:HG3	1.93	0.68
1:D:63:GLN:HB3	1:D:64:PRO:HD3	1.75	0.68
1:A:136:LEU:O	1:A:139:VAL:HG22	1.92	0.68
1:C:156:ARG:HD2	1:C:231:GLU:OE2	1.94	0.68
1:B:223:LYS:HB2	1:B:226:GLU:HG3	1.76	0.68
1:F:156:ARG:HD3	1:F:236:TYR:CG	2.29	0.68
1:C:156:ARG:HD3	1:C:236:TYR:CD2	2.29	0.68
1:A:156:ARG:HD2	1:A:231:GLU:OE2	1.94	0.67
1:A:166:TRP:HB3	1:A:190:ILE:HD11	1.76	0.67
1:C:199:GLN:NE2	3:C:22:SO4:O2	2.27	0.67
1:C:63:GLN:HB3	1:C:64:PRO:HD3	1.76	0.67
1:E:156:ARG:HD3	1:E:236:TYR:CD2	2.30	0.66
1:B:170:LYS:O	1:B:173:ILE:HD12	1.96	0.66
1:F:204:ARG:NH1	1:F:222:MET:HE3	2.10	0.66
1:C:159:VAL:O	1:C:163:GLU:HG3	1.95	0.65
1:B:238:ASN:HD21	2:B:500:MET:N	1.95	0.65
1:B:173:ILE:H	1:B:173:ILE:HD13	1.63	0.64
1:B:200:LEU:HD12	4:B:461:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:ARG:HD2	1:E:231:GLU:OE2	1.97	0.64
1:B:253:LYS:O	1:B:257:GLU:HG3	1.97	0.64
1:B:147:ALA:HB1	1:B:157:VAL:HG21	1.80	0.63
1:B:156:ARG:HD3	1:B:236:TYR:CG	2.34	0.63
1:F:204:ARG:CZ	1:F:222:MET:HE3	2.29	0.62
1:D:157:VAL:HG22	1:D:211:VAL:HG11	1.81	0.62
1:A:63:GLN:HB3	1:A:64:PRO:HD3	1.81	0.62
1:A:63:GLN:O	1:A:67:GLU:HG3	2.00	0.62
1:F:156:ARG:HD3	1:F:236:TYR:CD2	2.35	0.61
1:D:159:VAL:O	1:D:163:GLU:HG3	1.99	0.61
1:F:147:ALA:HB1	1:F:157:VAL:HG21	1.81	0.61
1:C:136:LEU:O	1:C:139:VAL:HG22	2.01	0.61
1:F:202:ARG:HG2	4:F:672:HOH:O	2.01	0.60
1:F:142:GLY:HA2	1:F:189:ASN:O	2.01	0.60
1:F:126:LEU:HD11	1:F:211:VAL:HG12	1.84	0.59
1:E:63:GLN:HB3	1:E:64:PRO:CD	2.33	0.59
1:A:130:PRO:HG3	1:A:228:LEU:HD21	1.83	0.59
1:D:44:GLU:HG3	1:D:72:THR:CG2	2.33	0.58
1:D:200:LEU:HD13	1:D:211:VAL:O	2.04	0.58
1:F:63:GLN:HB3	1:F:64:PRO:HD3	1.85	0.58
1:D:271:ARG:NH2	4:D:922:HOH:O	2.37	0.58
1:D:142:GLY:HA2	1:D:191:LYS:HE2	1.86	0.57
1:C:276:LYS:HD2	4:C:331:HOH:O	2.03	0.57
1:D:134:LYS:HD2	1:D:134:LYS:N	2.20	0.57
1:C:104:LEU:HD22	1:C:108:LYS:HD2	1.87	0.57
1:D:121:VAL:O	1:D:123:THR:HG22	2.04	0.57
1:A:144:THR:HG22	1:A:191:LYS:HB2	1.87	0.57
1:B:156:ARG:HD3	1:B:236:TYR:CD2	2.38	0.56
1:A:159:VAL:O	1:A:163:GLU:HG3	2.06	0.56
1:C:63:GLN:O	1:C:67:GLU:HG3	2.04	0.56
1:D:48:GLY:HA3	1:D:93:LEU:HD13	1.88	0.56
1:A:156:ARG:HD3	1:A:236:TYR:CD2	2.41	0.56
1:B:163:GLU:HG2	1:B:232:PRO:HG2	1.88	0.56
1:F:253:LYS:O	1:F:257:GLU:HG3	2.05	0.56
1:B:269:HIS:HE1	1:B:283:GLU:OE1	1.89	0.55
1:B:249:SER:HB2	3:B:3:SO4:O2	2.07	0.55
1:F:63:GLN:O	1:F:67:GLU:HG3	2.06	0.55
1:B:51:VAL:HG23	1:B:78:PHE:O	2.07	0.55
1:B:200:LEU:HD13	1:B:211:VAL:O	2.06	0.55
1:F:119:PHE:CD2	1:F:256:THR:HG22	2.42	0.55
1:D:67:GLU:HA	1:D:71:TYR:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ALA:HB1	1:D:157:VAL:HG21	1.89	0.55
1:F:95:ILE:HD11	1:F:240:SER:HB2	1.89	0.55
1:D:44:GLU:CG	1:D:72:THR:HG23	2.36	0.55
1:F:200:LEU:HD13	1:F:211:VAL:O	2.07	0.54
1:A:156:ARG:HD3	1:A:236:TYR:CG	2.42	0.54
1:B:180:LYS:HG2	4:B:808:HOH:O	2.07	0.54
1:E:136:LEU:O	1:E:139:VAL:CG2	2.55	0.54
1:E:200:LEU:HD13	1:E:211:VAL:O	2.08	0.54
1:F:104:LEU:HD22	1:F:108:LYS:HD3	1.88	0.54
1:A:166:TRP:HB3	1:A:190:ILE:HD12	1.90	0.53
1:F:238:ASN:N	1:F:238:ASN:HD22	2.05	0.53
1:F:156:ARG:HD3	1:F:236:TYR:CD1	2.43	0.53
1:C:108:LYS:O	1:C:112:ASN:N	2.41	0.53
1:E:276:LYS:HD2	4:E:312:HOH:O	2.08	0.53
1:F:86:LEU:O	1:F:90:GLU:HG3	2.08	0.53
1:C:59:LYS:NZ	1:C:63:GLN:HE22	2.06	0.53
1:C:101:LYS:HB3	1:C:102:PRO:HD3	1.91	0.53
1:C:61:GLN:C	1:C:64:PRO:HD2	2.35	0.52
1:C:156:ARG:HD3	1:C:236:TYR:CE2	2.44	0.52
1:D:154:PHE:CZ	1:D:180:LYS:HD2	2.44	0.52
1:D:173:ILE:HD12	1:D:173:ILE:C	2.35	0.52
1:E:136:LEU:O	1:E:139:VAL:HG22	2.10	0.52
1:E:252:LEU:O	1:E:256:THR:CG2	2.58	0.52
1:A:48:GLY:O	1:A:96:ASN:HA	2.10	0.51
1:C:104:LEU:O	1:C:108:LYS:HG3	2.10	0.51
1:B:251:TRP:O	1:B:255:VAL:HG23	2.11	0.51
1:B:173:ILE:H	1:B:173:ILE:CD1	2.23	0.51
1:A:223:LYS:HB2	1:A:226:GLU:HG3	1.93	0.51
1:A:276:LYS:HA	3:A:16:SO4:O3	2.10	0.51
1:F:200:LEU:HD12	4:F:306:HOH:O	2.10	0.51
1:F:119:PHE:HD2	1:F:256:THR:HG22	1.76	0.50
1:B:119:PHE:CD2	1:B:256:THR:HG22	2.46	0.50
1:F:130:PRO:HG3	1:F:228:LEU:HD21	1.94	0.50
1:F:100:HIS:CE1	1:F:103:TYR:HB2	2.47	0.50
1:D:238:ASN:N	1:D:238:ASN:HD22	2.09	0.50
1:E:223:LYS:HB2	1:E:226:GLU:HG3	1.94	0.50
1:A:108:LYS:HD2	1:A:115:ILE:O	2.11	0.50
1:B:248:ASP:O	1:B:249:SER:C	2.54	0.50
1:D:58:VAL:HA	1:D:62:ILE:HB	1.94	0.50
1:E:251:TRP:HD1	3:E:7:SO4:O2	1.95	0.49
1:F:148:PRO:HD2	1:F:157:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:ARG:HD3	1:E:236:TYR:CE2	2.47	0.49
1:B:154:PHE:HZ	1:B:180:LYS:HD3	1.77	0.49
1:C:84:PRO:HB2	1:C:98:PHE:CE2	2.48	0.49
1:E:108:LYS:HD2	1:E:115:ILE:O	2.13	0.49
1:F:139:VAL:HG22	1:F:209:PHE:CE2	2.47	0.49
1:C:156:ARG:HD3	1:C:236:TYR:CG	2.47	0.49
1:E:156:ARG:NH2	2:E:288:MET:OXT	2.42	0.49
1:E:251:TRP:O	1:E:255:VAL:HG23	2.13	0.49
1:F:201:PRO:HD2	4:F:672:HOH:O	2.11	0.49
1:C:86:LEU:O	1:C:90:GLU:HG3	2.14	0.48
1:B:48:GLY:HA3	1:B:93:LEU:HD13	1.94	0.48
1:F:120:GLN:HB2	1:F:278:PRO:HB3	1.95	0.48
1:F:156:ARG:NH2	2:F:288:MET:OXT	2.47	0.48
1:F:252:LEU:O	1:F:256:THR:HG23	2.12	0.48
1:F:223:LYS:HB2	1:F:226:GLU:HG3	1.95	0.48
1:B:156:ARG:HD3	1:B:236:TYR:CD1	2.47	0.48
1:C:156:ARG:NH2	2:C:400:MET:OXT	2.45	0.48
1:B:132:LYS:HE3	4:B:819:HOH:O	2.13	0.48
1:F:276:LYS:HD2	4:F:31:HOH:O	2.14	0.48
1:A:184:ALA:C	1:A:185:GLU:HG3	2.39	0.47
1:C:136:LEU:O	1:C:139:VAL:CG2	2.62	0.47
1:D:123:THR:HG23	1:D:237:VAL:HG13	1.97	0.47
1:E:252:LEU:O	1:E:256:THR:HG22	2.14	0.47
1:D:59:LYS:HG3	1:D:75:LEU:HD22	1.96	0.46
1:A:136:LEU:O	1:A:139:VAL:CG2	2.62	0.46
1:B:50:THR:HG23	1:B:98:PHE:HB2	1.96	0.46
1:A:71:TYR:OH	1:A:254:ASP:OD2	2.28	0.46
1:C:67:GLU:C	1:C:69:LYS:H	2.22	0.46
1:C:238:ASN:N	1:C:238:ASN:HD22	2.13	0.46
1:D:249:SER:HB2	3:D:11:SO4:O2	2.15	0.46
1:C:147:ALA:HB1	1:C:157:VAL:HG21	1.98	0.46
1:A:193:VAL:HG13	1:C:77:GLU:OE1	2.16	0.46
1:A:271:ARG:HD3	1:D:112:ASN:O	2.16	0.46
1:A:157:VAL:HG22	1:A:211:VAL:HG11	1.97	0.46
1:B:55:GLY:HA3	1:B:77:GLU:OE2	2.16	0.46
1:D:144:THR:HG22	1:D:191:LYS:HB2	1.98	0.46
1:A:48:GLY:HA3	1:A:93:LEU:HD13	1.96	0.46
1:C:61:GLN:O	1:C:64:PRO:HD2	2.16	0.46
1:C:128:LEU:HD11	1:C:209:PHE:HB3	1.97	0.46
1:B:144:THR:HG22	1:B:191:LYS:HB2	1.99	0.45
1:A:197:ALA:HA	1:A:200:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ARG:O	1:B:271:ARG:HD3	2.16	0.45
1:F:202:ARG:HG2	1:F:202:ARG:H	1.35	0.45
1:B:48:GLY:O	1:B:96:ASN:HA	2.16	0.45
1:B:101:LYS:HB3	1:B:102:PRO:HD3	1.98	0.45
1:C:59:LYS:CE	1:C:63:GLN:HE22	2.30	0.45
1:F:126:LEU:HD11	1:F:211:VAL:CG1	2.47	0.45
1:A:238:ASN:N	1:A:238:ASN:HD22	2.14	0.45
1:B:154:PHE:CZ	1:B:180:LYS:HD3	2.52	0.45
1:F:166:TRP:HA	1:F:188:LYS:HG3	1.99	0.45
1:B:100:HIS:CE1	1:B:103:TYR:HB2	2.51	0.45
1:C:121:VAL:O	1:C:123:THR:HG22	2.17	0.45
1:C:253:LYS:O	1:C:257:GLU:HG2	2.17	0.45
1:E:100:HIS:CE1	1:E:103:TYR:HB2	2.52	0.45
1:B:156:ARG:NH2	2:B:500:MET:OXT	2.51	0.44
1:E:238:ASN:N	1:E:238:ASN:HD22	2.13	0.44
1:F:65:GLU:HG3	4:F:295:HOH:O	2.17	0.44
1:F:110:GLU:HG2	1:F:111:HIS:CD2	2.52	0.44
1:F:184:ALA:C	1:F:185:GLU:HG3	2.43	0.44
1:D:101:LYS:HB3	1:D:102:PRO:HD3	1.99	0.44
1:E:159:VAL:O	1:E:163:GLU:HG3	2.16	0.44
1:F:61:GLN:C	1:F:64:PRO:HD2	2.42	0.44
1:A:147:ALA:HB1	1:A:157:VAL:HG21	1.99	0.44
1:C:48:GLY:HA3	1:C:93:LEU:HD13	1.99	0.44
1:A:156:ARG:HD3	1:A:236:TYR:CD1	2.52	0.44
1:B:63:GLN:O	1:B:67:GLU:HG3	2.17	0.44
1:B:157:VAL:HG22	1:B:211:VAL:HG11	1.99	0.44
1:C:130:PRO:HG3	1:C:228:LEU:CD2	2.45	0.44
1:A:58:VAL:HA	1:A:62:ILE:HB	2.00	0.44
1:F:78:PHE:CD1	1:F:83:ARG:HB2	2.53	0.44
1:D:84:PRO:HB2	1:D:98:PHE:CE2	2.53	0.44
1:E:203:SER:O	1:E:207:VAL:HG22	2.17	0.44
1:F:136:LEU:O	1:F:139:VAL:HG23	2.18	0.43
1:C:271:ARG:O	1:C:271:ARG:HD3	2.18	0.43
1:A:84:PRO:HB2	1:A:98:PHE:CE2	2.53	0.43
1:F:232:PRO:HG2	4:F:663:HOH:O	2.19	0.43
1:B:95:ILE:HD11	1:B:240:SER:HB2	1.99	0.43
1:B:173:ILE:HD13	1:B:173:ILE:N	2.30	0.43
1:B:269:HIS:CE1	1:B:283:GLU:OE1	2.69	0.43
1:F:250:GLN:N	3:F:1:SO4:O2	2.51	0.43
1:D:251:TRP:O	1:D:255:VAL:HG23	2.19	0.43
1:E:86:LEU:O	1:E:90:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:ASP:HB3	1:D:60:GLU:OE2	2.19	0.43
1:D:203:SER:O	1:D:207:VAL:HG22	2.19	0.43
1:B:266:ALA:O	1:B:270:LYS:HG2	2.18	0.43
1:D:67:GLU:C	1:D:69:LYS:H	2.27	0.43
1:E:156:ARG:HD3	1:E:236:TYR:CG	2.54	0.43
1:F:48:GLY:O	1:F:96:ASN:HA	2.19	0.43
1:F:128:LEU:C	1:F:128:LEU:HD13	2.44	0.43
1:D:276:LYS:HA	3:D:12:SO4:O3	2.19	0.42
1:F:104:LEU:HD21	1:F:108:LYS:HD3	2.00	0.42
1:A:51:VAL:HG22	1:A:52:GLY:N	2.34	0.42
1:F:135:SER:C	1:F:137:GLU:H	2.27	0.42
1:B:119:PHE:CE2	1:B:256:THR:HG22	2.54	0.42
1:E:119:PHE:CD2	1:E:256:THR:HB	2.55	0.42
1:A:128:LEU:CD1	1:A:128:LEU:C	2.92	0.42
1:C:168:LYS:HB3	1:C:185:GLU:HB2	2.01	0.42
1:B:147:ALA:CB	1:B:157:VAL:HG21	2.49	0.42
1:A:156:ARG:HD3	1:A:236:TYR:CE2	2.54	0.42
1:C:58:VAL:HA	1:C:62:ILE:HB	2.00	0.42
1:B:148:PRO:HD3	1:B:200:LEU:HD11	2.01	0.42
1:C:100:HIS:CE1	1:C:103:TYR:HB2	2.55	0.42
1:D:154:PHE:HZ	1:D:180:LYS:HD2	1.84	0.42
1:F:135:SER:C	1:F:137:GLU:N	2.77	0.41
1:F:168:LYS:HB3	1:F:185:GLU:HB2	2.02	0.41
1:F:83:ARG:HG2	1:F:83:ARG:H	1.65	0.41
1:C:249:SER:HB2	3:C:13:SO4:O2	2.19	0.41
1:D:100:HIS:CE1	1:D:103:TYR:HB2	2.56	0.41
1:F:130:PRO:HB3	1:F:134:LYS:HA	2.02	0.41
1:E:189:ASN:ND2	3:E:17:SO4:O4	2.53	0.41
1:B:84:PRO:HB2	1:B:98:PHE:CE2	2.56	0.41
1:B:237:VAL:HG21	4:B:833:HOH:O	2.21	0.41
1:E:170:LYS:HG3	1:E:182:ASP:O	2.21	0.41
1:F:139:VAL:HG22	1:F:209:PHE:CZ	2.55	0.41
1:F:62:ILE:HG13	1:F:259:TYR:CZ	2.55	0.41
1:F:66:LEU:O	1:F:71:TYR:HB2	2.21	0.41
1:F:238:ASN:N	1:F:238:ASN:ND2	2.69	0.41
1:C:61:GLN:NE2	1:C:65:GLU:OE2	2.36	0.40
1:F:249:SER:HB2	3:F:1:SO4:O2	2.21	0.40
1:D:147:ALA:O	1:D:194:GLU:HA	2.22	0.40
1:E:128:LEU:HD13	1:E:211:VAL:HG22	2.03	0.40
1:E:71:TYR:OH	1:E:251:TRP:HA	2.21	0.40
1:E:120:GLN:HB2	1:E:278:PRO:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:LEU:HD22	1:C:108:LYS:CD	2.50	0.40
1:D:271:ARG:HG2	4:D:617:HOH:O	2.22	0.40
1:E:141:ASP:HA	1:E:188:LYS:O	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	237/245 (97%)	231 (98%)	5 (2%)	1 (0%)	30	26
1	B	242/245 (99%)	233 (96%)	7 (3%)	2 (1%)	16	10
1	C	237/245 (97%)	230 (97%)	6 (2%)	1 (0%)	30	26
1	D	237/245 (97%)	234 (99%)	2 (1%)	1 (0%)	30	26
1	E	237/245 (97%)	231 (98%)	5 (2%)	1 (0%)	30	26
1	F	242/245 (99%)	231 (96%)	9 (4%)	2 (1%)	16	10
All	All	1432/1470 (97%)	1390 (97%)	34 (2%)	8 (1%)	21	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	249	SER
1	C	98	PHE
1	E	98	PHE
1	F	98	PHE
1	A	98	PHE
1	B	98	PHE
1	D	98	PHE
1	F	187	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	202/206 (98%)	195 (96%)	7 (4%)	32	32
1	B	205/206 (100%)	200 (98%)	5 (2%)	43	47
1	C	202/206 (98%)	194 (96%)	8 (4%)	28	27
1	D	202/206 (98%)	192 (95%)	10 (5%)	22	18
1	E	202/206 (98%)	193 (96%)	9 (4%)	24	22
1	F	204/206 (99%)	192 (94%)	12 (6%)	18	13
All	All	1217/1236 (98%)	1166 (96%)	51 (4%)	26	25

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	88	LEU
1	A	104	LEU
1	A	128	LEU
1	A	137	GLU
1	A	139	VAL
1	A	271	ARG
1	B	88	LEU
1	B	104	LEU
1	B	139	VAL
1	B	173	ILE
1	B	253	LYS
1	C	50	THR
1	C	88	LEU
1	C	104	LEU
1	C	108	LYS
1	C	114	ASP
1	C	123	THR
1	C	139	VAL
1	C	257	GLU
1	D	50	THR
1	D	64	PRO

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Mol	Chain	Res	Type
1	D	92	GLU
1	D	104	LEU
1	D	106	ASP
1	D	123	THR
1	D	128	LEU
1	D	134	LYS
1	D	180	LYS
1	D	185	GLU
1	E	88	LEU
1	E	104	LEU
1	E	108	LYS
1	E	134	LYS
1	E	135	SER
1	E	139	VAL
1	E	140	LYS
1	E	173	ILE
1	E	256	THR
1	F	50	THR
1	F	72	THR
1	F	74	LYS
1	F	79	THR
1	F	84	PRO
1	F	88	LEU
1	F	104	LEU
1	F	110	GLU
1	F	112	ASN
1	F	171	ASP
1	F	202	ARG
1	F	248	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	ASN
1	B	189	ASN
1	B	269	HIS
1	C	63	GLN
1	C	111	HIS
1	C	213	ASN
1	C	238	ASN
1	D	61	GLN
1	D	63	GLN

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Mol	Chain	Res	Type
1	D	112	ASN
1	D	189	ASN
1	D	199	GLN
1	D	213	ASN
1	D	238	ASN
1	E	238	ASN
1	F	111	HIS
1	F	189	ASN
1	F	215	ASN
1	F	238	ASN
1	F	269	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	MET	A	600	-	7,8,8	0.80	0	5,9,9	0.23	0
3	SO4	D	12	-	4,4,4	0.29	0	6,6,6	0.14	0
3	SO4	E	17	-	4,4,4	0.31	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	E	6	-	4,4,4	0.29	0	6,6,6	0.09	0
2	MET	E	288	-	7,8,8	0.75	0	5,9,9	0.27	0
2	MET	B	500	-	7,8,8	0.77	0	5,9,9	0.18	0
2	MET	F	288	-	7,8,8	0.75	0	5,9,9	0.26	0
3	SO4	A	16	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	D	11	-	4,4,4	0.28	0	6,6,6	0.07	0
3	SO4	A	15	-	4,4,4	0.31	0	6,6,6	0.09	0
3	SO4	C	2	-	4,4,4	0.32	0	6,6,6	0.07	0
3	SO4	C	5	-	4,4,4	0.24	0	6,6,6	0.05	0
3	SO4	B	19	-	4,4,4	0.32	0	6,6,6	0.05	0
3	SO4	C	20	-	4,4,4	0.33	0	6,6,6	0.03	0
3	SO4	F	1	-	4,4,4	0.29	0	6,6,6	0.07	0
2	MET	C	400	-	7,8,8	0.81	0	5,9,9	0.19	0
3	SO4	C	22	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	18	-	4,4,4	0.30	0	6,6,6	0.04	0
3	SO4	B	3	-	4,4,4	0.30	0	6,6,6	0.08	0
3	SO4	C	13	-	4,4,4	0.28	0	6,6,6	0.07	0
3	SO4	E	4	-	4,4,4	0.27	0	6,6,6	0.06	0
3	SO4	D	21	-	4,4,4	0.28	0	6,6,6	0.06	0
3	SO4	E	7	-	4,4,4	0.27	0	6,6,6	0.09	0
2	MET	D	300	-	7,8,8	0.78	0	5,9,9	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
2	MET	A	600	-	-	0/8/8/8	-
2	MET	C	400	-	-	0/8/8/8	-
2	MET	B	500	-	-	0/8/8/8	-
2	MET	F	288	-	-	1/8/8/8	-
2	MET	D	300	-	-	0/8/8/8	-
2	MET	E	288	-	-	0/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	288	MET	OXT-C-CA-N

There are no ring outliers.

13 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	12	SO4	1	0
3	E	17	SO4	1	0
2	E	288	MET	1	0
2	B	500	MET	2	0
2	F	288	MET	1	0
3	A	16	SO4	1	0
3	D	11	SO4	1	0
3	F	1	SO4	2	0
2	C	400	MET	1	0
3	C	22	SO4	1	0
3	B	3	SO4	1	0
3	C	13	SO4	1	0
3	E	7	SO4	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	239/245 (97%)	-0.38	0 100 100	12, 20, 32, 35	0
1	B	244/245 (99%)	-0.00	5 (2%) 65 69	14, 23, 42, 52	0
1	C	239/245 (97%)	-0.12	5 (2%) 63 67	14, 23, 40, 47	0
1	D	239/245 (97%)	-0.08	4 (1%) 69 73	16, 24, 41, 52	0
1	E	239/245 (97%)	-0.18	1 (0%) 88 90	13, 22, 41, 48	0
1	F	244/245 (99%)	0.77	31 (12%) 8 8	17, 34, 52, 62	0
All	All	1444/1470 (98%)	0.00	46 (3%) 50 54	12, 24, 43, 62	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	ASP	4.7
1	F	109	LYS	4.4
1	F	139	VAL	4.3
1	B	286	ALA	4.3
1	F	112	ASN	3.5
1	C	269	HIS	3.4
1	C	43	LYS	3.2
1	F	43	LYS	3.0
1	F	271	ARG	2.9
1	F	248	ASP	2.8
1	B	256	THR	2.8
1	B	269	HIS	2.8
1	C	140	LYS	2.8
1	F	247	LYS	2.7
1	F	72	THR	2.7
1	D	269	HIS	2.7
1	E	269	HIS	2.7
1	F	111	HIS	2.7
1	F	269	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	110	GLU	2.6
1	F	107	PHE	2.6
1	F	48	GLY	2.6
1	F	65	GLU	2.6
1	F	45	ILE	2.6
1	F	137	GLU	2.6
1	F	74	LYS	2.5
1	F	64	PRO	2.5
1	D	72	THR	2.5
1	F	168	LYS	2.5
1	F	286	ALA	2.4
1	F	202	ARG	2.4
1	F	256	THR	2.4
1	F	113	LEU	2.4
1	F	70	GLY	2.3
1	F	185	GLU	2.3
1	F	136	LEU	2.3
1	F	58	VAL	2.2
1	F	73	VAL	2.1
1	C	72	THR	2.1
1	F	91	GLY	2.1
1	F	92	GLU	2.1
1	F	171	ASP	2.1
1	D	273	GLU	2.1
1	B	273	GLU	2.0
1	F	184	ALA	2.0
1	C	112	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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(Å ²)	Q<0.9
3	SO4	F	1	5/5	0.64	0.21	89,89,90,90	0
3	SO4	D	11	5/5	0.66	0.27	82,83,83,83	0
3	SO4	E	17	5/5	0.66	0.23	75,76,77,77	0
3	SO4	B	18	5/5	0.66	0.18	77,78,78,79	0
3	SO4	D	21	5/5	0.76	0.15	74,75,75,76	0
3	SO4	A	16	5/5	0.77	0.21	81,81,81,82	0
3	SO4	C	22	5/5	0.77	0.20	72,73,73,74	0
3	SO4	B	3	5/5	0.78	0.20	63,64,65,66	0
3	SO4	B	19	5/5	0.78	0.15	74,74,75,75	0
3	SO4	D	12	5/5	0.78	0.21	92,92,92,92	0
3	SO4	E	7	5/5	0.79	0.17	69,69,70,71	0
3	SO4	C	2	5/5	0.80	0.18	78,79,79,79	0
3	SO4	C	13	5/5	0.83	0.15	80,81,81,81	0
3	SO4	C	20	5/5	0.86	0.18	66,66,67,68	0
3	SO4	E	6	5/5	0.86	0.15	81,81,82,82	0
3	SO4	C	5	5/5	0.89	0.19	55,57,58,59	0
3	SO4	E	4	5/5	0.93	0.14	36,40,42,42	0
3	SO4	A	15	5/5	0.98	0.07	32,34,35,36	0
2	MET	A	600	9/9	0.98	0.05	11,13,14,15	0
2	MET	B	500	9/9	0.98	0.06	11,13,15,17	0
2	MET	C	400	9/9	0.98	0.06	12,14,14,15	0
2	MET	D	300	9/9	0.98	0.05	10,14,17,17	0
2	MET	F	288	9/9	0.98	0.05	16,18,19,20	0
2	MET	E	288	9/9	0.99	0.04	10,14,16,16	0

6.5 Other polymers

There are no such residues in this entry.