



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:31 AM UTC

PDB ID : 5ZMM / pdb_00005zmm
Title : Structure of the Type IV phosphorothioation-dependent restriction endonuclease ScoMcrA
Authors : Liu, G.; Fu, W.; Zhang, Z.; He, Y.; Yu, H.; Zhao, Y.; Deng, Z.; Wu, G.; He, X.
Deposited on : 2018-04-04
Resolution : 3.15 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

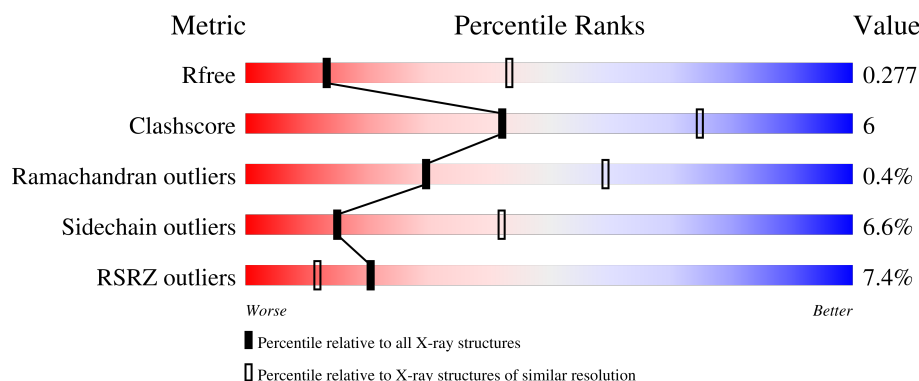
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	561	3% 74% 18% 6%
1	B	561	5% 73% 19% 6%
1	C	561	6% 76% 15% 7%
1	D	561	12% 71% 14% 13%
1	E	561	12% 74% 14% 11%

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Mol	Chain	Length	Quality of chain
1	F	561	2% 66% 15% 18%

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	ZN	A	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23352 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 Uncharacterized protein McrA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4089	2578	741	759	11			
1	B	527	Total	C	N	O	S	0	0	0
			4050	2552	735	752	11			
1	C	522	Total	C	N	O	S	0	0	0
			3972	2506	717	737	12			
1	D	489	Total	C	N	O	S	0	0	0
			3763	2374	692	686	11			
1	E	499	Total	C	N	O	S	0	0	0
			3812	2399	701	701	11			
1	F	462	Total	C	N	O	S	0	0	0
			3581	2255	655	660	11			

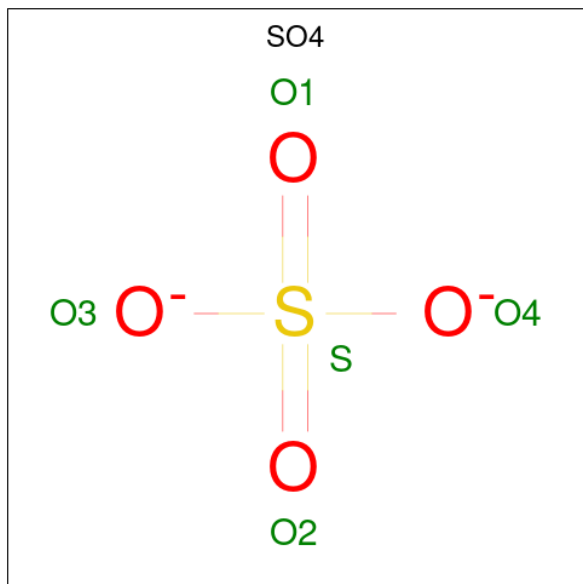
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q9L0M9
A	1	SER	-	expression tag	UNP Q9L0M9
B	0	GLY	-	expression tag	UNP Q9L0M9
B	1	SER	-	expression tag	UNP Q9L0M9
C	0	GLY	-	expression tag	UNP Q9L0M9
C	1	SER	-	expression tag	UNP Q9L0M9
D	0	GLY	-	expression tag	UNP Q9L0M9
D	1	SER	-	expression tag	UNP Q9L0M9
E	0	GLY	-	expression tag	UNP Q9L0M9
E	1	SER	-	expression tag	UNP Q9L0M9
F	0	GLY	-	expression tag	UNP Q9L0M9
F	1	SER	-	expression tag	UNP Q9L0M9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	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	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		

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

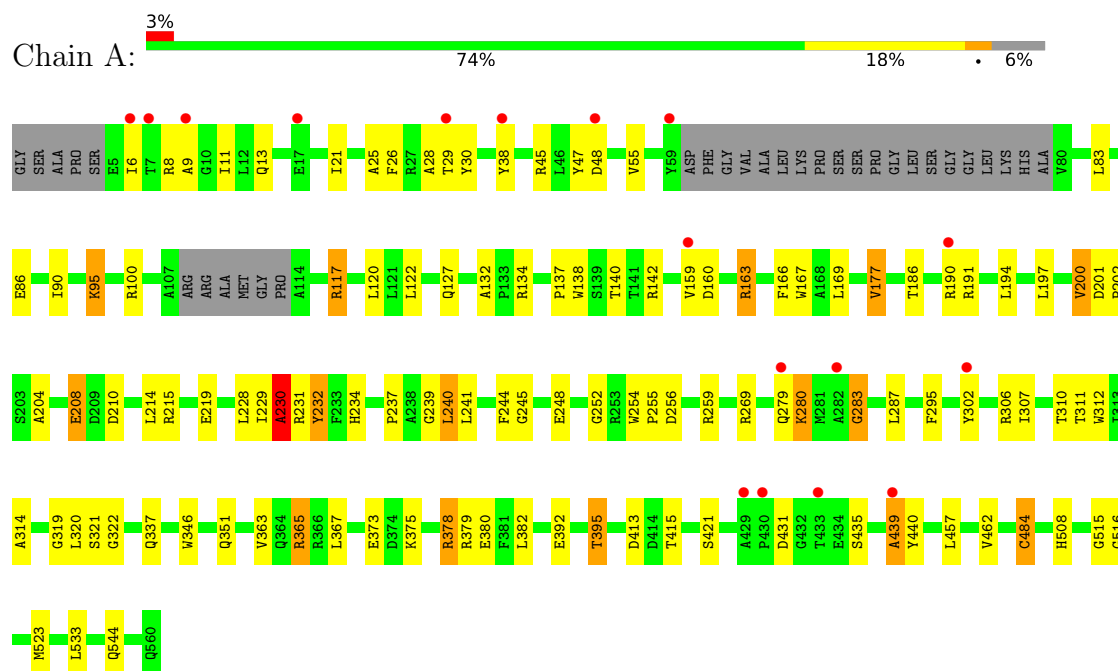
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	5	Total	O	0	0
			5	5		
4	C	5	Total	O	0	0
			5	5		
4	D	4	Total	O	0	0
			4	4		
4	F	3	Total	O	0	0
			3	3		

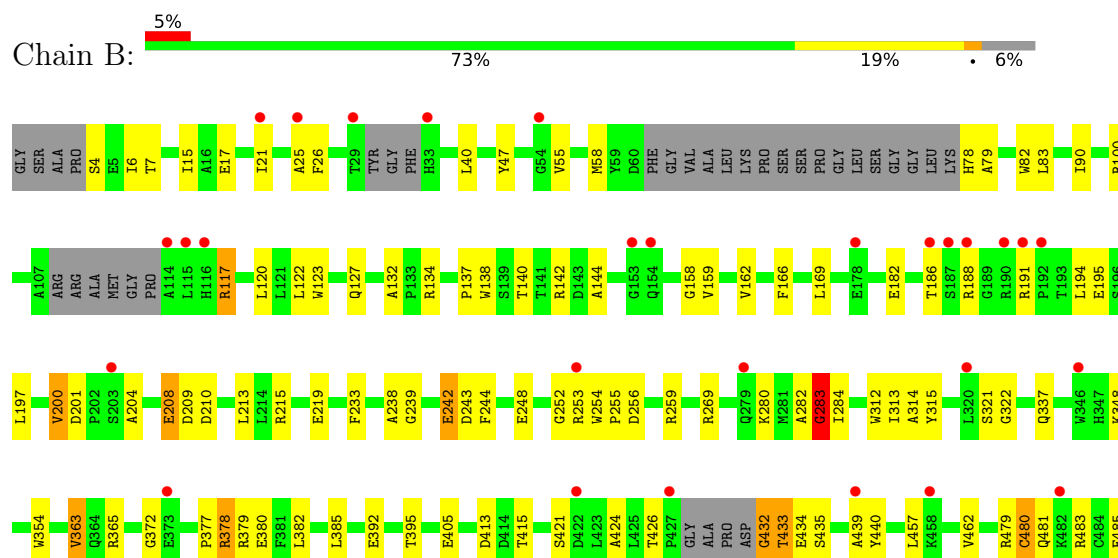
3 Residue-property plots

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: Uncharacterized protein McrA

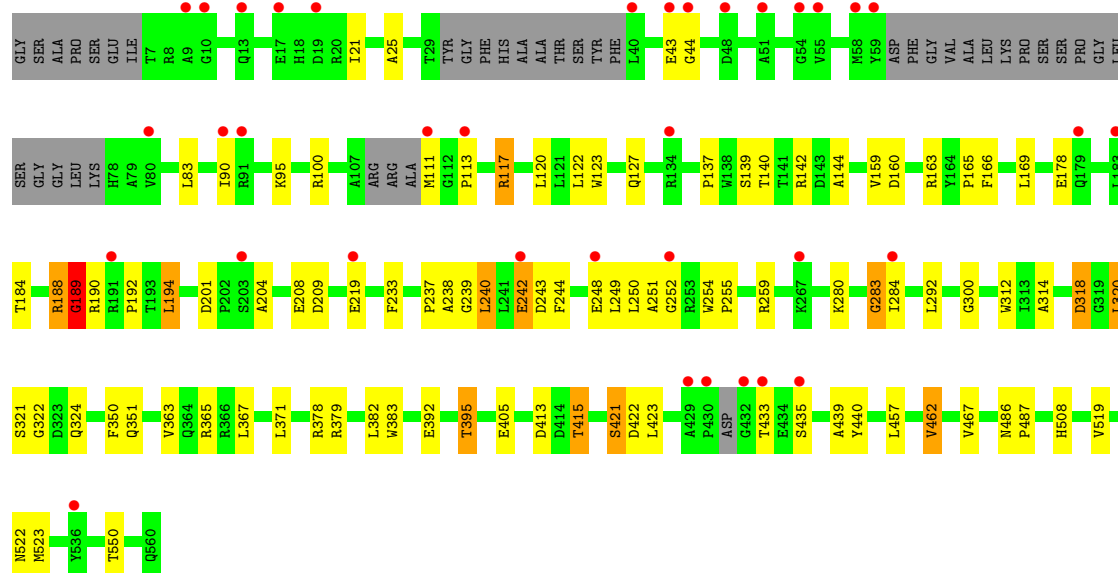
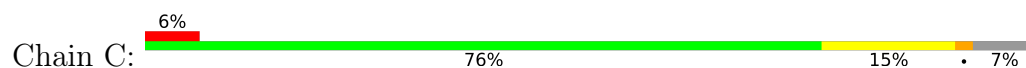


• Molecule 1: Uncharacterized protein McrA

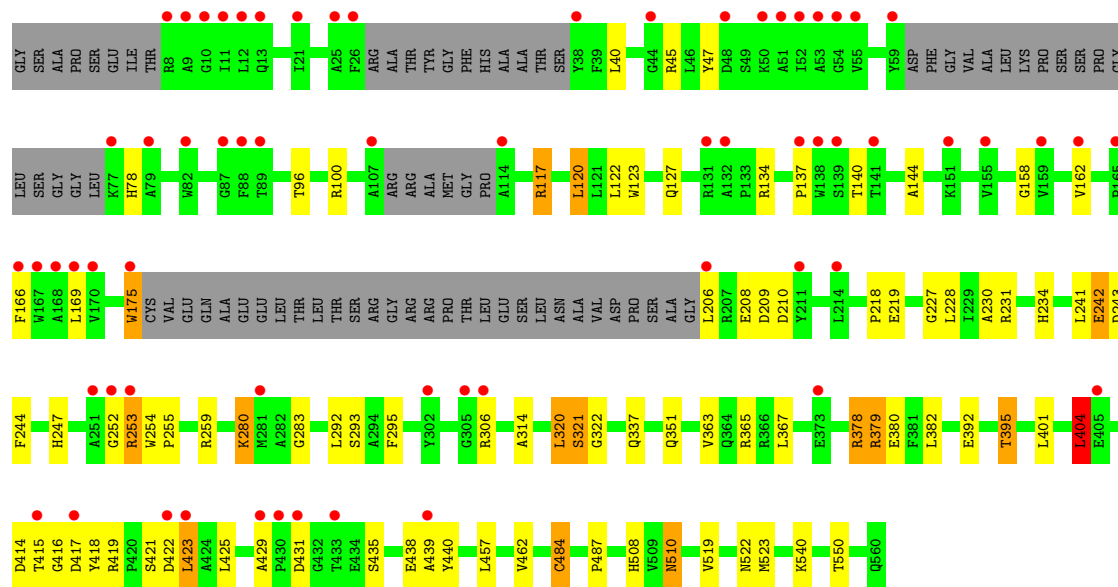




• Molecule 1: Uncharacterized protein McrA

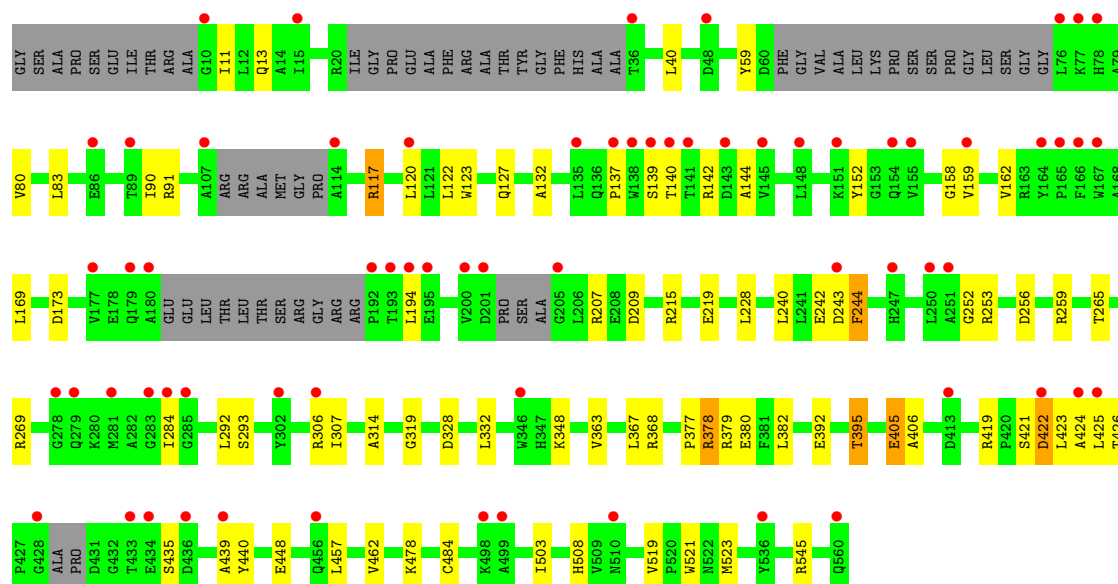


• Molecule 1: Uncharacterized protein McrA

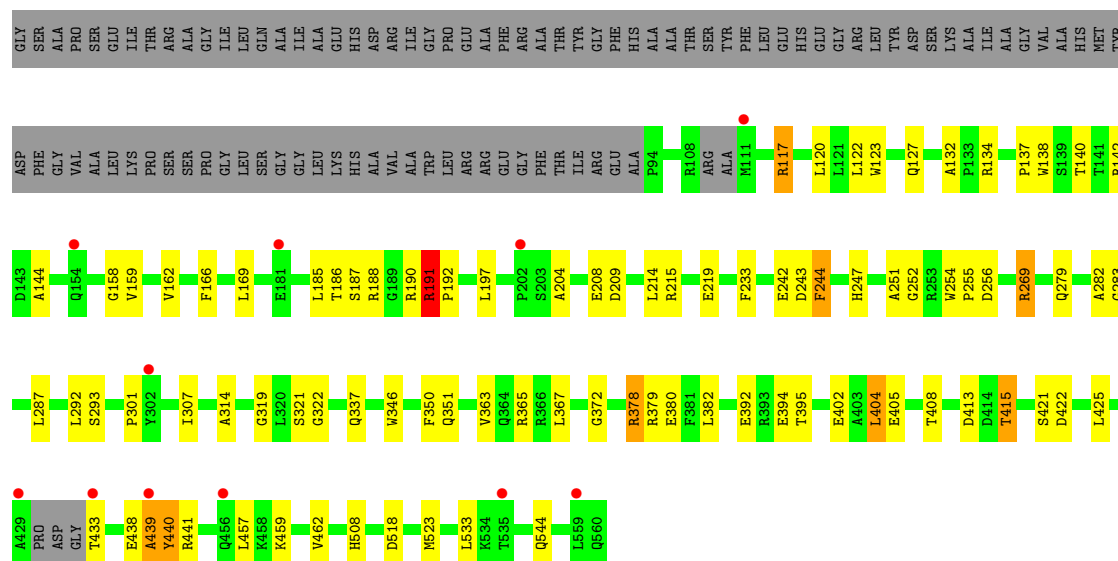


• Molecule 1: Uncharacterized protein McrA





• Molecule 1: Uncharacterized protein McrA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.18Å 139.37Å 281.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	140.50 – 3.15 140.50 – 3.15	Depositor EDS
% Data completeness (in resolution range)	88.2 (140.50-3.15) 88.3 (140.50-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.245 , 0.280 0.245 , 0.277	Depositor DCC
R_{free} test set	3796 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23352	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: SO4, ZN

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	2/4190 (0.0%)	1.06	4/5705 (0.1%)
1	B	0.91	5/4148 (0.1%)	1.08	15/5648 (0.3%)
1	C	0.96	4/4070 (0.1%)	1.10	11/5547 (0.2%)
1	D	0.89	2/3856 (0.1%)	1.07	9/5242 (0.2%)
1	E	0.84	0/3899	1.02	6/5299 (0.1%)
1	F	0.87	1/3670 (0.0%)	1.05	10/4996 (0.2%)
All	All	0.90	14/23833 (0.1%)	1.06	55/32437 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	7
1	D	0	4
1	E	0	1
1	F	0	3
All	All	0	24

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	433	THR	N-CA	8.68	1.57	1.46
1	C	189	GLY	N-CA	6.60	1.54	1.45
1	B	480	CYS	CA-C	-6.40	1.45	1.52
1	D	321	SER	N-CA	6.18	1.54	1.46
1	C	190	ARG	N-CA	6.17	1.54	1.46
1	B	284	ILE	CA-C	6.04	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	439	ALA	CA-C	5.42	1.61	1.52
1	D	320	LEU	N-CA	5.37	1.52	1.46
1	C	188	ARG	CA-C	5.30	1.59	1.52
1	F	243	ASP	N-CA	5.27	1.53	1.46
1	C	486	ASN	CA-C	-5.22	1.47	1.52
1	A	230	ALA	N-CA	5.08	1.52	1.46
1	B	432	GLY	CA-C	5.04	1.61	1.52
1	B	481	GLN	CA-C	-5.03	1.46	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	422	ASP	N-CA-C	-12.78	97.79	113.50
1	B	433	THR	N-CA-C	-12.33	96.74	112.90
1	F	405	GLU	N-CA-C	-12.12	96.96	112.23
1	C	422	ASP	N-CA-C	-11.89	98.75	113.38
1	F	243	ASP	N-CA-C	-9.95	100.55	112.89
1	A	320	LEU	N-CA-C	9.32	124.44	112.89
1	B	284	ILE	N-CA-C	-8.90	98.18	109.30
1	D	404	LEU	N-CA-C	-8.77	95.39	109.76
1	C	188	ARG	N-CA-C	8.32	120.26	111.03
1	B	200	VAL	N-CA-C	-8.15	98.13	108.89
1	A	240	LEU	N-CA-C	-7.89	98.13	109.96
1	E	244	PHE	N-CA-C	7.70	122.25	113.01
1	D	242	GLU	N-CA-C	-7.34	96.44	108.41
1	B	239	GLY	N-CA-C	7.16	130.14	113.18
1	B	421	SER	N-CA-C	6.82	118.79	107.20
1	C	242	GLU	N-CA-C	-6.64	96.20	108.02
1	A	232	TYR	N-CA-C	6.51	124.66	110.80
1	C	190	ARG	N-CA-C	-6.37	104.76	113.30
1	D	439	ALA	CA-C-N	6.32	133.08	121.70
1	D	439	ALA	C-N-CA	6.32	133.08	121.70
1	F	439	ALA	CA-C-N	6.31	133.05	121.70
1	F	439	ALA	C-N-CA	6.31	133.05	121.70
1	B	242	GLU	N-CA-C	-6.22	96.95	108.02
1	E	422	ASP	CB-CA-C	-6.15	103.14	112.11
1	B	421	SER	CB-CA-C	-6.10	103.87	111.43
1	F	191	ARG	N-CA-C	6.00	113.41	108.07
1	F	233	PHE	N-CA-C	5.98	119.89	112.24
1	B	233	PHE	N-CA-C	5.97	119.88	112.24
1	B	283	GLY	N-CA-C	-5.78	101.27	112.02
1	B	242	GLU	CA-C-N	5.77	132.08	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	GLU	C-N-CA	5.77	132.08	121.70
1	F	404	LEU	N-CA-C	-5.71	105.06	111.28
1	B	243	ASP	N-CA-C	5.68	126.91	111.00
1	A	200	VAL	CB-CA-C	-5.62	104.15	110.96
1	C	320	LEU	N-CA-C	5.59	118.31	111.82
1	C	283	GLY	N-CA-C	5.58	121.06	112.81
1	D	243	ASP	N-CA-C	5.57	126.61	111.00
1	E	405	GLU	N-CA-C	-5.49	102.16	110.28
1	B	480	CYS	O-C-N	5.41	129.54	123.27
1	D	242	GLU	CA-C-N	5.38	131.38	121.70
1	D	242	GLU	C-N-CA	5.38	131.38	121.70
1	C	318	ASP	N-CA-C	-5.36	102.07	110.17
1	D	404	LEU	CA-C-O	-5.36	114.85	120.80
1	C	243	ASP	N-CA-C	5.35	125.99	111.00
1	C	44	GLY	N-CA-C	-5.35	107.89	115.43
1	C	423	LEU	CB-CA-C	5.34	118.34	109.53
1	E	422	ASP	CA-C-O	-5.30	115.40	122.03
1	F	440	TYR	N-CA-CB	5.25	119.42	110.50
1	B	479	ARG	CA-C-N	-5.18	115.70	123.00
1	B	479	ARG	C-N-CA	-5.18	115.70	123.00
1	C	233	PHE	N-CA-C	5.05	118.70	112.24
1	D	418	TYR	CB-CA-C	5.05	118.03	111.42
1	F	244	PHE	N-CA-C	5.03	119.26	113.18
1	E	422	ASP	CA-C-N	5.02	130.73	121.70
1	E	422	ASP	C-N-CA	5.02	130.73	121.70

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	ARG	Peptide
1	A	239	GLY	Peptide
1	A	245	GLY	Peptide
1	A	283	GLY	Peptide
1	A	439	ALA	Peptide
1	B	238	ALA	Peptide
1	B	283	GLY	Peptide
1	B	432	GLY	Peptide
1	B	439	ALA	Peptide
1	C	188	ARG	Peptide
1	C	189	GLY	Peptide
1	C	242	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	C	320	LEU	Peptide
1	C	421	SER	Peptide
1	C	43	GLU	Peptide
1	C	439	ALA	Peptide
1	D	241	LEU	Peptide
1	D	320	LEU	Peptide
1	D	423	LEU	Peptide
1	D	438	GLU	Peptide
1	E	439	ALA	Peptide
1	F	242	GLU	Peptide
1	F	404	LEU	Peptide
1	F	438	GLU	Peptide

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	4089	0	3944	66	0
1	B	4050	0	3886	51	0
1	C	3972	0	3795	43	0
1	D	3763	0	3618	53	0
1	E	3812	0	3647	45	0
1	F	3581	0	3480	48	0
2	A	1	0	0	2	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	1	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	10	0	0	0	0
3	B	5	0	0	1	0
3	C	15	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	1	0
3	F	10	0	0	0	0
4	A	7	0	0	0	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	4	0	0	1	0
4	F	3	0	0	0	0
All	All	23352	0	22370	288	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 6.

All (288) 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:A:484:CYS:HG	2:A:601:ZN:ZN	0.68	0.90
1:D:253:ARG:HG3	1:D:255:PRO:HD2	1.51	0.89
1:C:283:GLY:HA2	1:C:284:ILE:O	1.81	0.80
1:D:414:ASP:OD1	1:D:415:THR:N	2.18	0.77
1:E:422:ASP:CB	1:E:478:LYS:HE2	2.16	0.76
1:F:279:GLN:HB2	1:F:282:ALA:HB2	1.68	0.75
1:C:252:GLY:HA2	1:D:219:GLU:HB3	1.69	0.75
1:C:283:GLY:CA	1:C:284:ILE:C	2.60	0.75
1:B:413:ASP:OD1	1:B:415:THR:OG1	2.05	0.74
1:C:283:GLY:HA2	1:C:284:ILE:C	2.15	0.72
1:A:252:GLY:HA2	1:B:219:GLU:HB3	1.70	0.72
1:B:197:LEU:O	1:B:200:VAL:O	2.08	0.71
1:A:252:GLY:CA	1:B:219:GLU:HB3	2.22	0.69
1:A:200:VAL:O	1:A:202:PRO:HD3	1.93	0.69
1:A:197:LEU:O	1:A:200:VAL:O	2.11	0.68
1:D:419:ARG:O	1:D:422:ASP:CB	2.41	0.68
1:E:423:LEU:HD23	1:E:424:ALA:C	2.20	0.67
1:A:484:CYS:SG	2:A:601:ZN:ZN	1.80	0.67
1:E:252:GLY:CA	1:F:219:GLU:HB3	2.25	0.67
1:C:142:ARG:HD3	1:C:159:VAL:HG13	1.78	0.66
1:D:484:CYS:SG	2:D:601:ZN:ZN	1.85	0.66
1:A:392:GLU:O	1:A:395:THR:HG22	1.96	0.65
1:F:142:ARG:HD3	1:F:159:VAL:HG13	1.78	0.65
1:B:392:GLU:O	1:B:395:THR:HG22	1.95	0.65
1:F:413:ASP:OD1	1:F:415:THR:HB	1.96	0.65
1:D:401:LEU:O	1:D:404:LEU:O	2.15	0.65
1:D:392:GLU:O	1:D:395:THR:HG22	1.97	0.64
1:A:142:ARG:HD3	1:A:159:VAL:HG13	1.80	0.64
1:E:142:ARG:HD3	1:E:159:VAL:HG13	1.79	0.64
1:E:219:GLU:HB3	1:F:252:GLY:HA2	1.79	0.64
1:E:252:GLY:HA3	1:F:219:GLU:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:LYS:O	1:D:280:LYS:HD3	1.99	0.63
1:D:367:LEU:O	1:D:414:ASP:HB3	1.97	0.63
1:A:269:ARG:HG2	1:A:280:LYS:HG2	1.80	0.62
1:A:413:ASP:OD1	1:A:415:THR:OG1	2.16	0.62
1:A:160:ASP:OD1	1:A:163:ARG:NH2	2.32	0.62
1:A:230:ALA:N	1:A:231:ARG:O	2.33	0.62
1:B:142:ARG:HD3	1:B:159:VAL:HG13	1.82	0.61
1:F:269:ARG:NH1	1:F:283:GLY:H	1.98	0.61
1:D:253:ARG:HG3	1:D:255:PRO:CD	2.28	0.61
1:F:314:ALA:HB1	1:F:382:LEU:HD11	1.84	0.60
1:E:269:ARG:N	3:E:602:SO4:O1	2.35	0.59
1:B:269:ARG:HH21	1:B:282:ALA:HA	1.68	0.58
1:A:219:GLU:HB3	1:B:252:GLY:HA2	1.85	0.57
1:C:252:GLY:CA	1:D:219:GLU:HB3	2.35	0.57
1:A:117:ARG:HG2	1:A:169:LEU:HD13	1.87	0.57
1:D:414:ASP:HA	4:D:702:HOH:O	2.04	0.57
1:C:413:ASP:OD1	1:C:415:THR:HB	2.05	0.56
1:D:314:ALA:HB1	1:D:382:LEU:HD11	1.88	0.56
1:E:219:GLU:HB3	1:F:252:GLY:CA	2.36	0.56
1:A:219:GLU:HB3	1:B:252:GLY:CA	2.36	0.56
1:F:392:GLU:O	1:F:395:THR:HG22	2.06	0.56
1:E:392:GLU:O	1:E:395:THR:HG22	2.06	0.55
1:E:377:PRO:HG3	1:E:426:THR:HG21	1.87	0.55
1:A:166:PHE:CZ	1:A:204:ALA:HB3	2.41	0.55
1:B:166:PHE:CZ	1:B:204:ALA:HB3	2.42	0.55
1:B:79:ALA:HA	1:B:82:TRP:CE3	2.41	0.55
1:F:137:PRO:HG2	1:F:140:THR:HG22	1.89	0.55
1:B:186:THR:HG22	1:B:188:ARG:H	1.72	0.55
1:D:242:GLU:HG2	1:D:247:HIS:HB2	1.88	0.54
1:A:137:PRO:HG2	1:A:140:THR:HG22	1.89	0.54
1:C:237:PRO:HD2	1:C:240:LEU:HD23	1.89	0.54
1:A:279:GLN:HE21	1:A:280:LYS:H	1.56	0.54
1:A:367:LEU:HD21	1:A:379:ARG:HG2	1.90	0.54
1:E:423:LEU:HD23	1:E:425:LEU:N	2.23	0.54
1:C:318:ASP:O	1:C:324:GLN:NE2	2.40	0.53
1:C:209:ASP:OD1	1:C:209:ASP:N	2.41	0.53
1:D:252:GLY:O	1:D:253:ARG:NH1	2.41	0.53
1:A:279:GLN:NE2	1:A:280:LYS:H	2.06	0.53
1:C:392:GLU:O	1:C:395:THR:HG22	2.07	0.53
1:A:283:GLY:HA3	1:A:295:PHE:HB2	1.90	0.53
1:B:283:GLY:HA2	1:B:315:TYR:OH	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ARG:HD3	1:C:194:LEU:HG	1.92	0.52
1:C:137:PRO:HG2	1:C:140:THR:HG22	1.90	0.52
1:F:166:PHE:CZ	1:F:204:ALA:HB3	2.44	0.52
1:C:123:TRP:CH2	1:C:144:ALA:HB1	2.44	0.52
1:E:252:GLY:HA2	1:F:219:GLU:HB3	1.91	0.52
1:E:319:GLY:O	1:E:378:ARG:NH2	2.43	0.52
1:E:314:ALA:HB1	1:E:382:LEU:HD11	1.92	0.52
1:A:186:THR:HG23	1:A:191:ARG:O	2.10	0.52
1:C:166:PHE:CZ	1:C:204:ALA:HB3	2.44	0.52
1:B:132:ALA:O	1:B:215:ARG:NH2	2.43	0.51
1:B:321:SER:HB2	1:B:372:GLY:HA3	1.91	0.51
1:D:416:GLY:O	1:D:417:ASP:CB	2.57	0.51
1:C:314:ALA:HB1	1:C:382:LEU:HD11	1.93	0.51
1:A:508:HIS:NE2	1:A:523:MET:HE2	2.26	0.51
1:E:367:LEU:HD21	1:E:379:ARG:HG2	1.92	0.51
1:B:314:ALA:HB1	1:B:382:LEU:HD11	1.94	0.50
1:C:163:ARG:NH1	1:C:192:PRO:O	2.44	0.50
1:D:510:ASN:HB2	1:D:522:ASN:OD1	2.11	0.50
1:A:132:ALA:O	1:A:215:ARG:NH2	2.44	0.50
1:A:319:GLY:O	1:A:378:ARG:NH2	2.44	0.50
1:D:166:PHE:HA	1:D:175:TRP:HZ3	1.76	0.50
1:B:209:ASP:OD1	1:B:209:ASP:N	2.45	0.50
1:C:350:PHE:CD2	1:C:351:GLN:HG3	2.46	0.50
1:E:132:ALA:O	1:E:215:ARG:NH2	2.44	0.50
1:F:117:ARG:HG2	1:F:169:LEU:HD13	1.93	0.50
1:B:137:PRO:HG2	1:B:140:THR:HG22	1.94	0.50
1:F:132:ALA:O	1:F:215:ARG:NH2	2.45	0.50
1:F:319:GLY:O	1:F:378:ARG:NH2	2.45	0.50
1:A:252:GLY:HA3	1:B:219:GLU:HB3	1.93	0.50
1:F:321:SER:HB2	1:F:372:GLY:HA3	1.93	0.50
1:A:228:LEU:O	1:A:231:ARG:O	2.30	0.49
1:B:17:GLU:O	1:B:21:ILE:HG22	2.12	0.49
1:A:314:ALA:HB1	1:A:382:LEU:HD11	1.94	0.49
1:E:13:GLN:CB	1:E:59:TYR:CE2	2.95	0.49
1:E:378:ARG:NH1	1:E:380:GLU:OE1	2.45	0.49
1:B:100:ARG:NH2	1:B:210:ASP:OD2	2.46	0.49
1:D:230:ALA:O	1:D:234:HIS:HB3	2.13	0.49
1:D:280:LYS:HD3	1:D:280:LYS:C	2.36	0.49
1:E:137:PRO:HG2	1:E:140:THR:HG22	1.95	0.49
1:B:158:GLY:O	1:B:162:VAL:HG23	2.13	0.49
1:B:242:GLU:HA	1:B:244:PHE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:GLU:O	1:E:406:ALA:HB3	2.12	0.49
1:C:160:ASP:O	1:C:163:ARG:HG3	2.13	0.49
1:D:401:LEU:C	1:D:404:LEU:O	2.56	0.49
1:A:30:TYR:CD2	1:A:55:VAL:HG22	2.48	0.49
1:B:424:ALA:HB3	1:B:501:LEU:HD22	1.95	0.49
1:C:322:GLY:O	1:C:378:ARG:HD2	2.12	0.48
1:E:240:LEU:O	1:E:244:PHE:HD1	1.94	0.48
1:A:26:PHE:CZ	1:A:55:VAL:HG21	2.49	0.48
1:E:122:LEU:HB3	1:E:244:PHE:CE2	2.48	0.48
1:B:117:ARG:HG2	1:B:169:LEU:HD13	1.95	0.48
1:C:117:ARG:HG2	1:C:169:LEU:HD13	1.95	0.48
1:D:429:ALA:HB3	1:D:431:ASP:N	2.29	0.48
1:D:519:VAL:O	1:D:523:MET:HG3	2.13	0.48
1:E:256:ASP:HB3	1:F:256:ASP:HB3	1.96	0.48
1:C:283:GLY:HA3	1:C:284:ILE:C	2.37	0.48
1:C:300:GLY:HA2	1:C:350:PHE:CE1	2.48	0.48
1:D:137:PRO:HG2	1:D:140:THR:HG22	1.94	0.48
1:E:158:GLY:O	1:E:162:VAL:HG23	2.14	0.48
1:A:302:TYR:CG	1:A:302:TYR:O	2.67	0.47
1:B:269:ARG:N	3:B:602:SO4:O3	2.42	0.47
1:F:367:LEU:HD21	1:F:379:ARG:HG2	1.95	0.47
1:A:134:ARG:NH2	1:A:208:GLU:HA	2.30	0.47
1:A:256:ASP:HB3	1:B:256:ASP:HB3	1.96	0.47
1:B:348:LYS:HD3	1:B:354:TRP:CD1	2.50	0.47
1:D:242:GLU:HG2	1:D:247:HIS:CB	2.43	0.47
1:A:21:ILE:HG22	1:A:25:ALA:HB3	1.97	0.47
1:B:134:ARG:NH2	1:B:208:GLU:HA	2.29	0.47
1:C:367:LEU:HD21	1:C:379:ARG:HG2	1.97	0.47
1:E:209:ASP:OD1	1:E:209:ASP:N	2.47	0.47
1:F:269:ARG:HH12	1:F:283:GLY:H	1.63	0.47
1:A:508:HIS:HE2	1:A:523:MET:HE2	1.79	0.47
1:E:242:GLU:HA	1:E:243:ASP:C	2.39	0.47
1:F:508:HIS:NE2	1:F:523:MET:HE2	2.30	0.47
1:B:480:CYS:SG	1:B:483:ARG:HB2	2.56	0.46
1:B:21:ILE:HG13	1:B:25:ALA:HB3	1.96	0.46
1:B:378:ARG:HD3	1:B:380:GLU:HB3	1.97	0.46
1:B:517:PRO:HD2	1:B:522:ASN:ND2	2.31	0.46
1:F:187:SER:O	1:F:188:ARG:CB	2.64	0.46
1:E:448:GLU:OE2	1:E:521:TRP:NE1	2.44	0.46
1:F:378:ARG:HD3	1:F:380:GLU:HB3	1.97	0.46
1:A:322:GLY:C	1:A:378:ARG:HG3	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:PRO:HG3	1:C:550:THR:HG21	1.98	0.46
1:B:377:PRO:HG3	1:B:426:THR:HG21	1.97	0.46
1:C:21:ILE:HG22	1:C:25:ALA:HB3	1.97	0.46
1:E:378:ARG:HD3	1:E:380:GLU:HB3	1.97	0.46
1:A:287:LEU:HD21	1:A:346:TRP:CH2	2.52	0.45
1:E:328:ASP:O	1:E:332:LEU:HD13	2.16	0.45
1:F:337:GLN:OE1	1:F:365:ARG:NH1	2.49	0.45
1:F:508:HIS:HE2	1:F:523:MET:HE2	1.80	0.45
1:D:120:LEU:HD11	1:D:175:TRP:CZ3	2.51	0.45
1:D:209:ASP:N	1:D:209:ASP:OD1	2.49	0.45
1:D:227:GLY:O	1:D:231:ARG:HD3	2.16	0.45
1:F:378:ARG:NH1	1:F:380:GLU:OE1	2.49	0.45
1:B:379:ARG:HG2	1:B:415:THR:HG21	1.97	0.45
1:A:337:GLN:OE1	1:A:365:ARG:NH1	2.50	0.45
1:A:45:ARG:HD3	1:A:47:TYR:OH	2.16	0.45
1:D:487:PRO:HG3	1:D:550:THR:HG21	1.99	0.45
1:E:152:TYR:CZ	1:E:240:LEU:HA	2.52	0.45
1:B:26:PHE:CZ	1:B:55:VAL:HG21	2.51	0.45
1:E:123:TRP:CH2	1:E:144:ALA:HB1	2.52	0.45
1:E:173:ASP:O	1:E:207:ARG:HD3	2.16	0.45
1:E:519:VAL:O	1:E:523:MET:HG3	2.17	0.45
1:A:8:ARG:O	1:A:9:ALA:HB3	2.18	0.45
1:A:229:ILE:O	1:A:230:ALA:C	2.60	0.45
1:F:191:ARG:HB2	1:F:192:PRO:HD2	1.99	0.45
1:B:337:GLN:OE1	1:B:365:ARG:NH1	2.49	0.44
1:B:508:HIS:NE2	1:B:523:MET:HE2	2.32	0.44
1:A:230:ALA:HB2	1:A:234:HIS:CB	2.47	0.44
1:D:508:HIS:NE2	1:D:523:MET:HE2	2.33	0.44
1:A:138:TRP:HB3	1:A:202:PRO:HD2	2.00	0.44
1:F:122:LEU:HB3	1:F:244:PHE:CE2	2.52	0.44
1:F:301:PRO:HD3	1:F:350:PHE:CE2	2.51	0.44
1:A:378:ARG:HG2	1:A:379:ARG:N	2.32	0.44
1:D:414:ASP:CG	1:D:415:THR:N	2.75	0.44
1:F:287:LEU:HD21	1:F:346:TRP:CH2	2.53	0.44
1:A:30:TYR:HD2	1:A:55:VAL:CG2	2.31	0.44
1:A:378:ARG:HD3	1:A:380:GLU:HB3	1.99	0.44
1:C:122:LEU:HB3	1:C:244:PHE:CE2	2.53	0.44
1:D:123:TRP:CH2	1:D:144:ALA:HB1	2.53	0.44
1:D:158:GLY:O	1:D:162:VAL:HG23	2.18	0.43
1:E:80:VAL:HG13	1:E:90:ILE:HD13	1.99	0.43
1:A:28:ALA:HA	1:A:29:THR:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:VAL:O	1:C:523:MET:HG3	2.17	0.43
1:E:117:ARG:HG2	1:E:169:LEU:HD13	2.00	0.43
1:A:100:ARG:NH2	1:A:210:ASP:OD2	2.50	0.43
1:B:322:GLY:C	1:B:378:ARG:HG3	2.43	0.43
1:D:100:ARG:NH2	1:D:210:ASP:OD2	2.50	0.43
1:D:134:ARG:NH2	1:D:208:GLU:HA	2.33	0.43
1:D:175:TRP:HE1	1:D:206:LEU:N	2.16	0.43
1:F:123:TRP:CH2	1:F:144:ALA:HB1	2.54	0.43
1:A:254:TRP:N	1:A:255:PRO:CD	2.81	0.43
1:F:209:ASP:OD1	1:F:209:ASP:N	2.50	0.43
1:A:95:LYS:O	1:A:100:ARG:HD3	2.18	0.43
1:D:166:PHE:HA	1:D:175:TRP:CZ3	2.53	0.43
1:A:373:GLU:O	1:A:375:LYS:HE2	2.19	0.43
1:D:337:GLN:OE1	1:D:365:ARG:NH1	2.52	0.43
1:D:421:SER:HA	1:D:423:LEU:N	2.34	0.43
1:E:503:ILE:CD1	1:F:533:LEU:HD23	2.49	0.43
1:B:254:TRP:CG	1:B:255:PRO:HD3	2.54	0.42
1:F:402:GLU:HB3	1:F:459:LYS:HE2	2.01	0.42
1:C:508:HIS:NE2	1:C:523:MET:HE2	2.34	0.42
1:D:292:LEU:HD23	1:D:293:SER:N	2.33	0.42
1:F:192:PRO:HG2	1:F:197:LEU:HD11	2.01	0.42
1:E:508:HIS:HE2	1:E:523:MET:HE2	1.85	0.42
1:D:120:LEU:HD11	1:D:175:TRP:HZ3	1.83	0.42
1:D:421:SER:HA	1:D:422:ASP:C	2.44	0.42
1:A:237:PRO:HD2	1:A:240:LEU:HD12	2.01	0.42
1:B:122:LEU:HB3	1:B:244:PHE:CE2	2.55	0.42
1:B:312:TRP:CZ3	1:B:363:VAL:HG11	2.55	0.42
1:D:254:TRP:N	1:D:255:PRO:CD	2.82	0.42
1:F:322:GLY:C	1:F:378:ARG:HG3	2.44	0.42
1:A:310:THR:HG22	1:A:312:TRP:H	1.85	0.42
1:B:15:ILE:HG23	1:B:47:TYR:CZ	2.55	0.42
1:B:83:LEU:HB2	1:B:90:ILE:HD11	2.01	0.42
1:B:123:TRP:CH2	1:B:144:ALA:HB1	2.55	0.42
1:F:254:TRP:CG	1:F:255:PRO:HD3	2.55	0.42
1:A:229:ILE:O	1:A:230:ALA:O	2.37	0.42
1:A:280:LYS:O	1:A:280:LYS:HD3	2.19	0.42
1:C:371:LEU:CD2	1:E:545:ARG:HD2	2.49	0.42
1:D:367:LEU:HD21	1:D:379:ARG:HG2	2.01	0.42
1:E:508:HIS:NE2	1:E:523:MET:HE2	2.35	0.42
1:F:392:GLU:OE1	1:F:394:GLU:HG3	2.19	0.42
1:D:378:ARG:HD3	1:D:380:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:ILE:HG22	1:E:314:ALA:HB2	2.02	0.42
1:F:508:HIS:NE2	1:F:518:ASP:OD1	2.44	0.42
1:C:83:LEU:HB2	1:C:90:ILE:HD11	2.01	0.42
1:D:283:GLY:O	1:D:295:PHE:HD1	2.02	0.42
1:A:167:TRP:CZ3	1:A:177:VAL:HG21	2.55	0.41
1:C:251:ALA:HB3	1:D:218:PRO:CG	2.50	0.41
1:C:254:TRP:N	1:C:255:PRO:CD	2.83	0.41
1:C:522:ASN:CG	1:C:522:ASN:O	2.63	0.41
1:A:8:ARG:CB	1:A:86:GLU:CB	2.98	0.41
1:B:117:ARG:NH1	4:B:701:HOH:O	2.47	0.41
1:C:312:TRP:CZ3	1:C:462:VAL:HG22	2.54	0.41
1:A:83:LEU:HB2	1:A:90:ILE:HD11	2.02	0.41
1:C:238:ALA:HA	1:C:239:GLY:HA2	1.84	0.41
1:F:186:THR:HG22	1:F:187:SER:N	2.35	0.41
1:E:378:ARG:HG2	1:E:379:ARG:N	2.34	0.41
1:B:313:ILE:HB	1:B:385:LEU:HB2	2.03	0.41
1:E:292:LEU:HD23	1:E:293:SER:N	2.35	0.41
1:C:95:LYS:O	1:C:100:ARG:HD3	2.21	0.41
1:C:139:SER:HB2	1:C:201:ASP:OD2	2.21	0.41
1:C:249:LEU:HG	1:C:250:LEU:HD13	2.03	0.41
1:C:433:THR:O	1:C:433:THR:HG22	2.19	0.41
1:A:122:LEU:HB3	1:A:244:PHE:CE2	2.56	0.41
1:A:307:ILE:HG22	1:A:314:ALA:HB2	2.01	0.41
1:E:419:ARG:O	1:E:421:SER:O	2.39	0.41
1:A:310:THR:HG22	1:A:311:THR:N	2.35	0.41
1:C:365:ARG:HD3	1:C:383:TRP:CZ3	2.56	0.41
1:E:11:ILE:HD13	1:E:83:LEU:HD23	2.03	0.41
1:E:421:SER:O	1:E:422:ASP:CB	2.69	0.41
1:F:138:TRP:CZ2	1:F:142:ARG:HG3	2.56	0.41
1:F:158:GLY:O	1:F:162:VAL:HG23	2.21	0.41
1:F:439:ALA:HA	1:F:441:ARG:H	1.86	0.41
1:A:177:VAL:HG12	1:A:204:ALA:HB2	2.03	0.41
1:B:138:TRP:CZ2	1:B:142:ARG:HG3	2.56	0.41
1:D:508:HIS:HE2	1:D:523:MET:HE2	1.85	0.41
1:F:134:ARG:NH2	1:F:208:GLU:HA	2.36	0.41
1:F:307:ILE:HG21	1:F:307:ILE:HD13	1.82	0.41
1:A:515:GLY:O	1:A:516:GLY:C	2.64	0.40
1:B:254:TRP:N	1:B:255:PRO:CD	2.84	0.40
1:D:122:LEU:HB3	1:D:244:PHE:CE2	2.56	0.40
1:D:322:GLY:C	1:D:378:ARG:HG3	2.47	0.40
1:A:11:ILE:HD13	1:A:83:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:ILE:CB	1:C:292:LEU:HD21	2.51	0.40
1:D:117:ARG:HG2	1:D:169:LEU:HD13	2.02	0.40
1:F:292:LEU:HD23	1:F:293:SER:N	2.36	0.40
1:F:254:TRP:N	1:F:255:PRO:CD	2.84	0.40
1:A:30:TYR:HD2	1:A:55:VAL:HG22	1.86	0.40
1:A:533:LEU:HD23	1:B:503:ILE:CD1	2.50	0.40
1:D:45:ARG:HB2	1:D:47:TYR:CE1	2.56	0.40
1:B:480:CYS:HB2	1:B:485:GLU:OE2	2.21	0.40
1:C:165:PRO:O	1:C:169:LEU:HB2	2.21	0.40
1:D:367:LEU:C	1:D:414:ASP:HB3	2.46	0.40
1:F:247:HIS:O	1:F:251:ALA:HB2	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	524/561 (93%)	489 (93%)	31 (6%)	4 (1%)	16	46
1	B	517/561 (92%)	487 (94%)	29 (6%)	1 (0%)	43	71
1	C	512/561 (91%)	486 (95%)	23 (4%)	3 (1%)	21	52
1	D	479/561 (85%)	451 (94%)	27 (6%)	1 (0%)	43	71
1	E	485/561 (86%)	461 (95%)	23 (5%)	1 (0%)	43	71
1	F	456/561 (81%)	431 (94%)	24 (5%)	1 (0%)	43	71
All	All	2973/3366 (88%)	2805 (94%)	157 (5%)	11 (0%)	30	59

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	TYR

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Mol	Chain	Res	Type
1	C	440	TYR
1	B	440	TYR
1	A	230	ALA
1	A	440	TYR
1	E	440	TYR
1	F	440	TYR
1	D	440	TYR
1	A	201	ASP
1	C	189	GLY
1	C	113	PRO

5.3.2 Protein sidechains [i](#)

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	403/440 (92%)	372 (92%)	31 (8%)	12	37
1	B	397/440 (90%)	368 (93%)	29 (7%)	13	38
1	C	386/440 (88%)	363 (94%)	23 (6%)	17	45
1	D	364/440 (83%)	338 (93%)	26 (7%)	13	40
1	E	367/440 (83%)	345 (94%)	22 (6%)	17	45
1	F	358/440 (81%)	339 (95%)	19 (5%)	20	49
All	All	2275/2640 (86%)	2125 (93%)	150 (7%)	15	42

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	13	GLN
1	A	38	TYR
1	A	48	ASP
1	A	95	LYS
1	A	117	ARG
1	A	120	LEU
1	A	127	GLN

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Mol	Chain	Res	Type
1	A	163	ARG
1	A	177	VAL
1	A	194	LEU
1	A	208	GLU
1	A	214	LEU
1	A	241	LEU
1	A	248	GLU
1	A	259	ARG
1	A	280	LYS
1	A	306	ARG
1	A	321	SER
1	A	351	GLN
1	A	363	VAL
1	A	365	ARG
1	A	378	ARG
1	A	395	THR
1	A	421	SER
1	A	431	ASP
1	A	435	SER
1	A	457	LEU
1	A	462	VAL
1	A	484	CYS
1	A	544	GLN
1	B	4	SER
1	B	6	ILE
1	B	7	THR
1	B	40	LEU
1	B	58	MET
1	B	78	HIS
1	B	117	ARG
1	B	120	LEU
1	B	127	GLN
1	B	182	GLU
1	B	191	ARG
1	B	194	LEU
1	B	195	GLU
1	B	201	ASP
1	B	208	GLU
1	B	213	LEU
1	B	248	GLU
1	B	253	ARG
1	B	259	ARG

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Mol	Chain	Res	Type
1	B	280	LYS
1	B	363	VAL
1	B	378	ARG
1	B	405	GLU
1	B	433	THR
1	B	434	GLU
1	B	435	SER
1	B	457	LEU
1	B	462	VAL
1	B	544	GLN
1	C	111	MET
1	C	117	ARG
1	C	120	LEU
1	C	127	GLN
1	C	178	GLU
1	C	184	THR
1	C	194	LEU
1	C	208	GLU
1	C	219	GLU
1	C	240	LEU
1	C	248	GLU
1	C	259	ARG
1	C	280	LYS
1	C	321	SER
1	C	363	VAL
1	C	395	THR
1	C	405	GLU
1	C	415	THR
1	C	421	SER
1	C	435	SER
1	C	457	LEU
1	C	462	VAL
1	C	467	VAL
1	D	40	LEU
1	D	78	HIS
1	D	96	THR
1	D	117	ARG
1	D	120	LEU
1	D	127	GLN
1	D	175	TRP
1	D	228	LEU
1	D	253	ARG

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Mol	Chain	Res	Type
1	D	259	ARG
1	D	280	LYS
1	D	306	ARG
1	D	321	SER
1	D	351	GLN
1	D	363	VAL
1	D	378	ARG
1	D	379	ARG
1	D	395	THR
1	D	404	LEU
1	D	425	LEU
1	D	435	SER
1	D	457	LEU
1	D	462	VAL
1	D	484	CYS
1	D	510	ASN
1	D	540	LYS
1	E	40	LEU
1	E	91	ARG
1	E	117	ARG
1	E	120	LEU
1	E	127	GLN
1	E	139	SER
1	E	194	LEU
1	E	228	LEU
1	E	253	ARG
1	E	259	ARG
1	E	265	THR
1	E	284	ILE
1	E	306	ARG
1	E	348	LYS
1	E	363	VAL
1	E	368	ARG
1	E	378	ARG
1	E	395	THR
1	E	435	SER
1	E	457	LEU
1	E	462	VAL
1	E	484	CYS
1	F	117	ARG
1	F	120	LEU
1	F	127	GLN

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Mol	Chain	Res	Type
1	F	185	LEU
1	F	190	ARG
1	F	191	ARG
1	F	214	LEU
1	F	269	ARG
1	F	351	GLN
1	F	363	VAL
1	F	378	ARG
1	F	408	THR
1	F	415	THR
1	F	421	SER
1	F	425	LEU
1	F	433	THR
1	F	457	LEU
1	F	462	VAL
1	F	544	GLN

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	127	GLN
1	A	212	ASN
1	A	279	GLN
1	A	510	ASN
1	B	127	GLN
1	B	179	GLN
1	B	510	ASN
1	C	127	GLN
1	C	510	ASN
1	D	127	GLN
1	D	212	ASN
1	D	450	ASN
1	D	555	HIS
1	E	279	GLN
1	E	353	GLN
1	E	555	HIS
1	F	127	GLN
1	F	179	GLN
1	F	212	ASN
1	F	510	ASN

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](#)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 for Mogul analysis.

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	$\# Z > 2$
3	SO4	A	602	-	4,4,4	0.46	0	6,6,6	0.76	0
3	SO4	C	603	-	4,4,4	0.57	0	6,6,6	0.69	0
3	SO4	C	602	-	4,4,4	0.55	0	6,6,6	0.83	0
3	SO4	E	602	-	4,4,4	0.33	0	6,6,6	0.52	0
3	SO4	B	602	-	4,4,4	0.58	0	6,6,6	0.29	0
3	SO4	D	603	-	4,4,4	0.70	0	6,6,6	0.52	0
3	SO4	A	603	-	4,4,4	0.48	0	6,6,6	0.27	0
3	SO4	D	602	-	4,4,4	0.59	0	6,6,6	0.32	0
3	SO4	F	602	-	4,4,4	0.50	0	6,6,6	0.55	0
3	SO4	C	604	-	4,4,4	0.57	0	6,6,6	0.83	0
3	SO4	F	603	-	4,4,4	0.59	0	6,6,6	0.90	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	602	SO4	1	0
3	B	602	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	530/561 (94%)	0.22	17 (3%)	50	30	33, 61, 97, 143	0
1	B	527/561 (93%)	0.38	29 (5%)	30	17	40, 69, 105, 132	0
1	C	522/561 (93%)	0.36	36 (6%)	23	13	30, 60, 117, 140	0
1	D	489/561 (87%)	0.69	65 (13%)	7	5	30, 71, 142, 173	0
1	E	499/561 (88%)	0.84	67 (13%)	7	4	30, 81, 148, 175	0
1	F	462/561 (82%)	0.23	11 (2%)	59	39	37, 63, 89, 121	0
All	All	3029/3366 (89%)	0.45	225 (7%)	20	12	30, 67, 126, 175	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	167	TRP	6.9
1	E	422	ASP	6.2
1	E	192	PRO	5.1
1	D	417	ASP	5.0
1	E	180	ALA	5.0
1	C	54	GLY	4.9
1	E	76	LEU	4.8
1	C	113	PRO	4.8
1	C	59	TYR	4.6
1	C	90	ILE	4.5
1	E	279	GLN	4.3
1	E	283	GLY	4.2
1	D	48	ASP	4.0
1	D	138	TRP	4.0
1	D	159	VAL	3.9
1	D	9	ALA	3.9
1	D	302	TYR	3.9
1	D	89	THR	3.8
1	A	302	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	10	GLY	3.8
1	D	13	GLN	3.7
1	B	279	GLN	3.7
1	C	432	GLY	3.7
1	D	44	GLY	3.7
1	C	48	ASP	3.7
1	D	59	TYR	3.6
1	D	429	ALA	3.6
1	E	560	GLN	3.6
1	C	58	MET	3.6
1	E	86	GLU	3.6
1	F	439	ALA	3.6
1	F	302	TYR	3.6
1	E	285	GLY	3.5
1	D	51	ALA	3.5
1	D	439	ALA	3.5
1	D	175	TRP	3.5
1	E	194	LEU	3.5
1	B	536	TYR	3.5
1	D	26	PHE	3.5
1	D	422	ASP	3.5
1	F	429	ALA	3.5
1	D	206	LEU	3.5
1	C	55	VAL	3.4
1	B	153	GLY	3.4
1	E	193	THR	3.4
1	D	87	GLY	3.4
1	C	111	MET	3.4
1	E	425	LEU	3.4
1	C	191	ARG	3.4
1	B	187	SER	3.4
1	A	429	ALA	3.4
1	D	21	ILE	3.4
1	E	250	LEU	3.3
1	A	6	ILE	3.3
1	C	430	PRO	3.3
1	E	281	MET	3.3
1	E	284	ILE	3.3
1	E	167	TRP	3.2
1	E	251	ALA	3.2
1	B	422	ASP	3.2
1	E	278	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	195	GLU	3.2
1	B	190	ARG	3.1
1	D	52	ILE	3.1
1	B	54	GLY	3.1
1	E	247	HIS	3.1
1	C	429	ALA	3.1
1	A	159	VAL	3.1
1	E	428	GLY	3.1
1	E	243	ASP	3.1
1	B	114	ALA	3.0
1	B	33	HIS	3.0
1	E	510	ASN	3.0
1	F	535	THR	3.0
1	C	10	GLY	3.0
1	E	141	THR	3.0
1	E	159	VAL	2.9
1	E	306	ARG	2.9
1	D	166	PHE	2.9
1	E	166	PHE	2.9
1	D	11	ILE	2.9
1	A	48	ASP	2.9
1	E	413	ASP	2.9
1	C	433	THR	2.9
1	E	201	ASP	2.8
1	C	91	ARG	2.8
1	C	17	GLU	2.8
1	F	456	GLN	2.8
1	A	29	THR	2.8
1	D	88	PHE	2.8
1	E	536	TYR	2.8
1	E	499	ALA	2.8
1	A	59	TYR	2.8
1	E	151	LYS	2.8
1	A	439	ALA	2.7
1	D	305	GLY	2.7
1	D	38	TYR	2.7
1	A	433	THR	2.7
1	E	140	THR	2.7
1	C	9	ALA	2.7
1	E	78	HIS	2.7
1	B	154	GLN	2.7
1	D	141	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	439	ALA	2.7
1	C	179	GLN	2.6
1	D	137	PRO	2.6
1	E	177	VAL	2.6
1	D	25	ALA	2.6
1	D	107	ALA	2.6
1	E	424	ALA	2.6
1	E	179	GLN	2.6
1	D	53	ALA	2.6
1	E	138	TRP	2.6
1	D	132	ALA	2.6
1	E	89	THR	2.6
1	E	433	THR	2.6
1	D	77	LYS	2.5
1	A	9	ALA	2.5
1	B	116	HIS	2.5
1	B	320	LEU	2.5
1	D	430	PRO	2.5
1	D	12	LEU	2.5
1	D	54	GLY	2.5
1	C	248	GLU	2.5
1	D	281	MET	2.5
1	A	7	THR	2.5
1	D	165	PRO	2.5
1	E	498	LYS	2.5
1	C	252	GLY	2.5
1	F	433	THR	2.5
1	C	134	ARG	2.5
1	E	107	ALA	2.4
1	C	43	GLU	2.4
1	E	36	THR	2.4
1	C	242	GLU	2.4
1	E	120	LEU	2.4
1	E	155	VAL	2.4
1	D	253	ARG	2.4
1	D	405	GLU	2.4
1	D	252	GLY	2.4
1	D	168	ALA	2.4
1	D	155	VAL	2.4
1	D	114	ALA	2.3
1	D	169	LEU	2.3
1	E	135	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	188	ARG	2.3
1	B	191	ARG	2.3
1	E	77	LYS	2.3
1	E	205	GLY	2.3
1	D	415	THR	2.3
1	E	148	LEU	2.3
1	B	482	LYS	2.3
1	D	50	LYS	2.3
1	D	8	ARG	2.3
1	B	346	TRP	2.3
1	F	154	GLN	2.3
1	D	170	VAL	2.3
1	D	306	ARG	2.3
1	D	10	GLY	2.3
1	C	536	TYR	2.3
1	C	219	GLU	2.2
1	E	137	PRO	2.2
1	F	202	PRO	2.2
1	E	114	ALA	2.2
1	E	439	ALA	2.2
1	A	38	TYR	2.2
1	E	139	SER	2.2
1	A	430	PRO	2.2
1	F	559	LEU	2.2
1	E	346	TRP	2.2
1	B	186	THR	2.2
1	C	435	SER	2.2
1	B	115	LEU	2.2
1	D	423	LEU	2.2
1	E	48	ASP	2.2
1	C	19	ASP	2.2
1	D	151	LYS	2.2
1	C	80	VAL	2.2
1	D	211	TYR	2.2
1	C	284	ILE	2.2
1	B	427	PRO	2.2
1	B	203	SER	2.1
1	A	190	ARG	2.1
1	E	15	ILE	2.1
1	E	302	TYR	2.1
1	C	13	GLN	2.1
1	E	456	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	111	MET	2.1
1	A	282	ALA	2.1
1	B	25	ALA	2.1
1	E	165	PRO	2.1
1	F	181	GLU	2.1
1	D	55	VAL	2.1
1	D	82	TRP	2.1
1	D	431	ASP	2.1
1	E	200	VAL	2.1
1	B	21	ILE	2.1
1	D	131	ARG	2.1
1	B	192	PRO	2.1
1	C	44	GLY	2.1
1	C	183	LEU	2.1
1	C	51	ALA	2.1
1	C	203	SER	2.1
1	D	139	SER	2.1
1	E	143	ASP	2.1
1	B	29	THR	2.1
1	A	279	GLN	2.1
1	B	373	GLU	2.1
1	D	373	GLU	2.1
1	C	267	LYS	2.0
1	D	214	LEU	2.0
1	D	79	ALA	2.0
1	D	433	THR	2.0
1	E	164	TYR	2.0
1	E	154	GLN	2.0
1	E	434	GLU	2.0
1	D	162	VAL	2.0
1	B	253	ARG	2.0
1	D	251	ALA	2.0
1	E	436	ASP	2.0
1	B	458	LYS	2.0
1	A	17	GLU	2.0
1	B	178	GLU	2.0
1	E	145	VAL	2.0
1	C	40	LEU	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 [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($\text{\AA}^2$)	Q<0.9
3	SO4	D	603	5/5	0.89	0.11	58,69,85,86	0
3	SO4	C	604	5/5	0.92	0.15	62,64,66,73	0
3	SO4	F	603	5/5	0.92	0.10	56,63,71,73	0
3	SO4	C	602	5/5	0.93	0.08	45,50,56,62	0
3	SO4	E	602	5/5	0.94	0.06	62,65,72,76	0
3	SO4	A	603	5/5	0.94	0.09	57,59,65,66	0
3	SO4	A	602	5/5	0.96	0.07	46,46,48,49	0
3	SO4	B	602	5/5	0.96	0.07	61,62,72,74	0
3	SO4	D	602	5/5	0.96	0.06	62,64,69,74	0
3	SO4	C	603	5/5	0.97	0.08	50,54,54,55	0
3	SO4	F	602	5/5	0.98	0.09	45,49,50,51	0
2	ZN	F	601	1/1	0.99	0.03	48,48,48,48	0
2	ZN	B	601	1/1	0.99	0.02	52,52,52,52	0
2	ZN	A	601	1/1	1.00	0.02	59,59,59,59	0
2	ZN	C	601	1/1	1.00	0.01	43,43,43,43	0
2	ZN	D	601	1/1	1.00	0.02	45,45,45,45	0
2	ZN	E	601	1/1	1.00	0.02	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.