



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 06:04 PM EDT

PDB ID : 3MM7
Title : Dissimilatory sulfite reductase carbon monoxide complex
Authors : Parey, K.; Warkentin, E.; Kroneck, P.M.H.; Ermler, U.
Deposited on : unknown
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

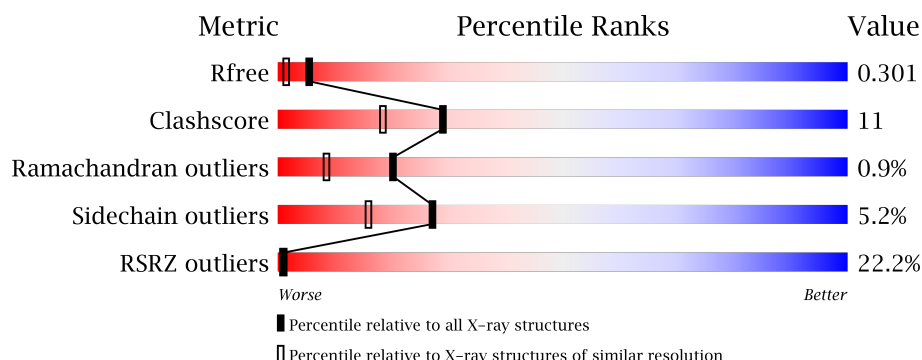
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	418	<div> <div>12%</div> <div>79%</div> <div>16%</div> <div>• •</div> </div>
1	D	418	<div> <div>28%</div> <div>84%</div> <div>15%</div> </div>
2	B	366	<div> <div>12%</div> <div>82%</div> <div>16%</div> <div>• • •</div> </div>
2	E	366	<div> <div>37%</div> <div>61%</div> <div>32%</div> <div>7%</div> <div>•</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	B	585	-	-	X	-
4	SF4	E	585	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13292 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.

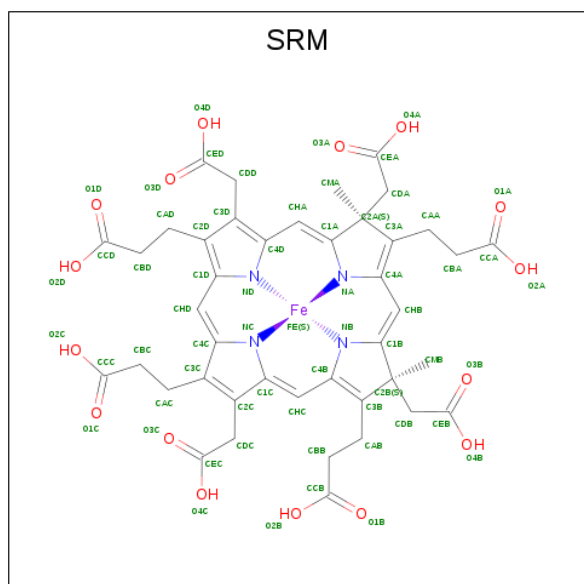
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3330	2134	557	613	26			
1	D	417	Total	C	N	O	S	0	0	0
			3330	2134	557	613	26			

- Molecule 2 is a protein called Sulfite reductase, dissimilatory-type subunit beta.

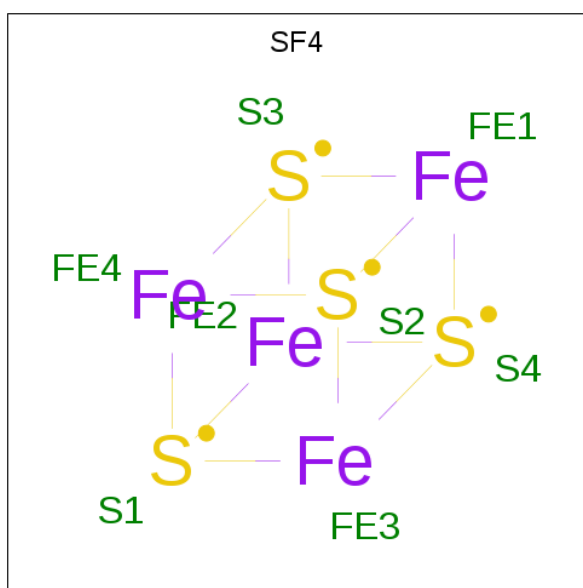
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			
2	E	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			

- Molecule 3 is SIROHEME (three-letter code: SRM) (formula: $C_{42}H_{42}FeN_4O_{16}$).



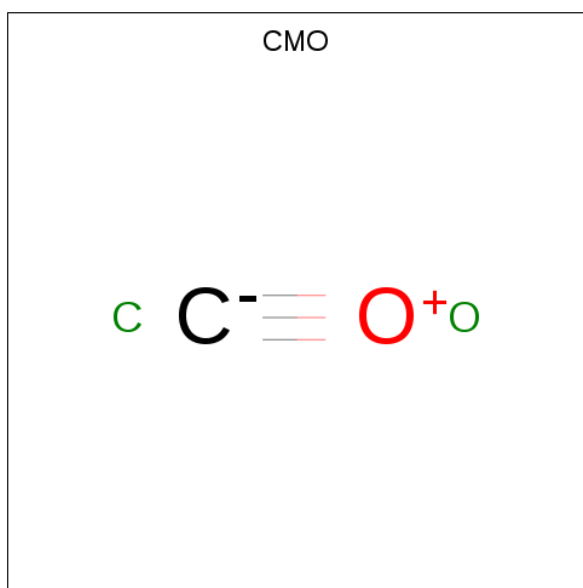
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	B	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	D	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	E	1	Total	C	Fe	N	O	
			63	42	1	4	16	

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S		
			8	4	4	0	0
4	A	1	Total	Fe	S		
			8	4	4	0	0
4	B	1	Total	Fe	S		
			8	4	4	0	0
4	B	1	Total	Fe	S		
			8	4	4	0	0
4	D	1	Total	Fe	S		
			8	4	4	0	0
4	D	1	Total	Fe	S		
			8	4	4	0	0
4	E	1	Total	Fe	S		
			8	4	4	0	0
4	E	1	Total	Fe	S		
			8	4	4	0	0

- Molecule 5 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			2	1	1		

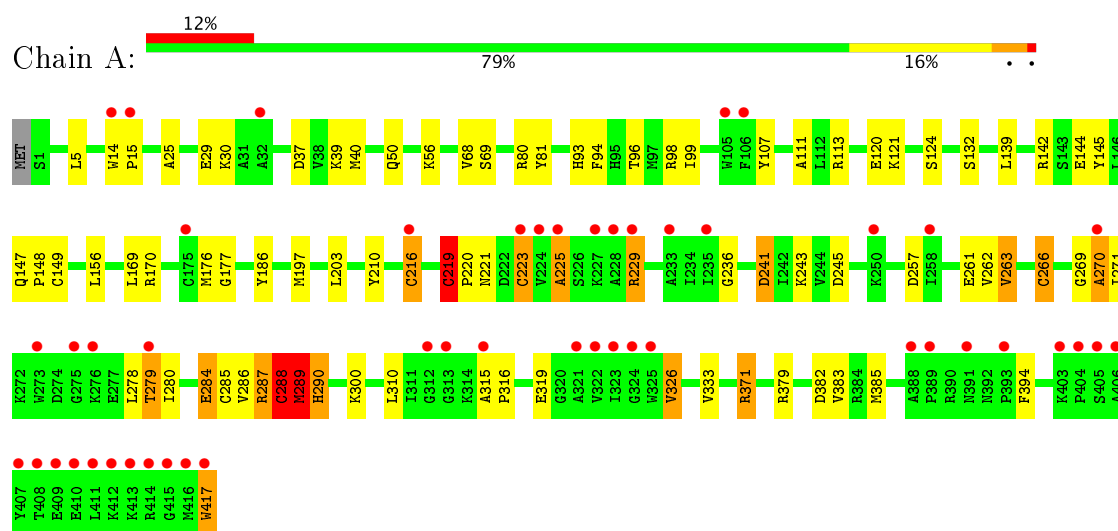
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	226	Total	O	0	0
			226	226		
6	B	209	Total	O	0	0
			209	209		
6	D	56	Total	O	0	0
			56	56		
6	E	21	Total	O	0	0
			21	21		

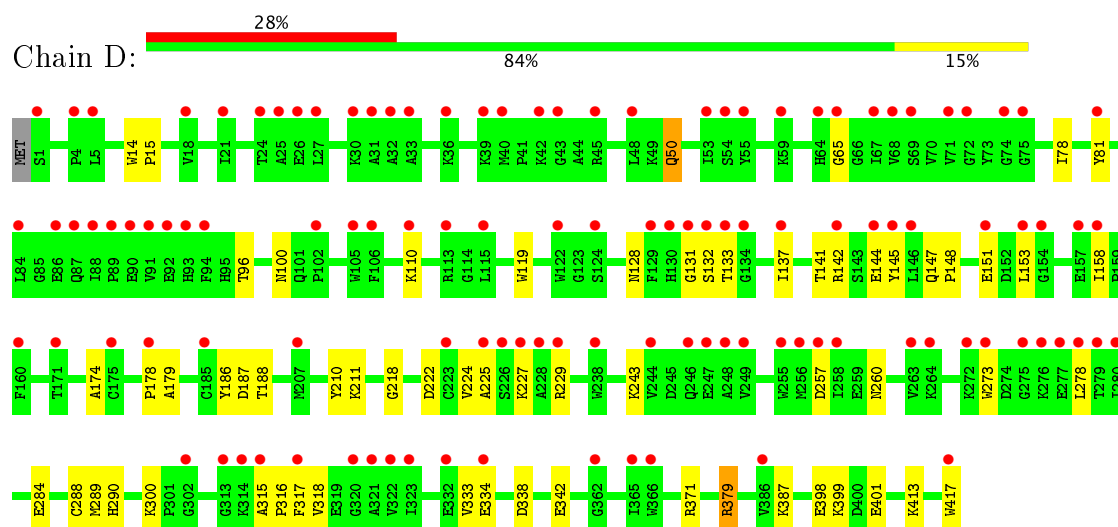
3 Residue-property plots [i](#)

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

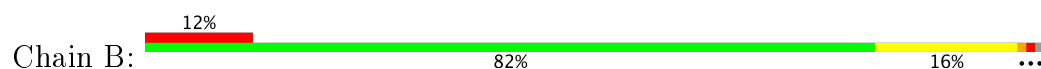
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

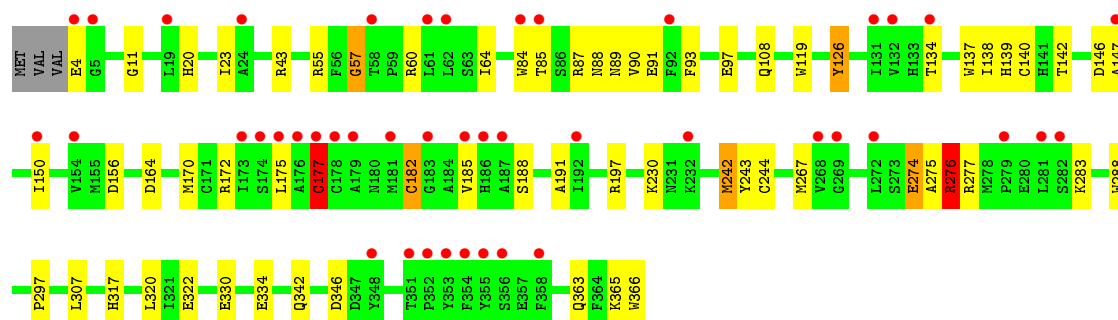


- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

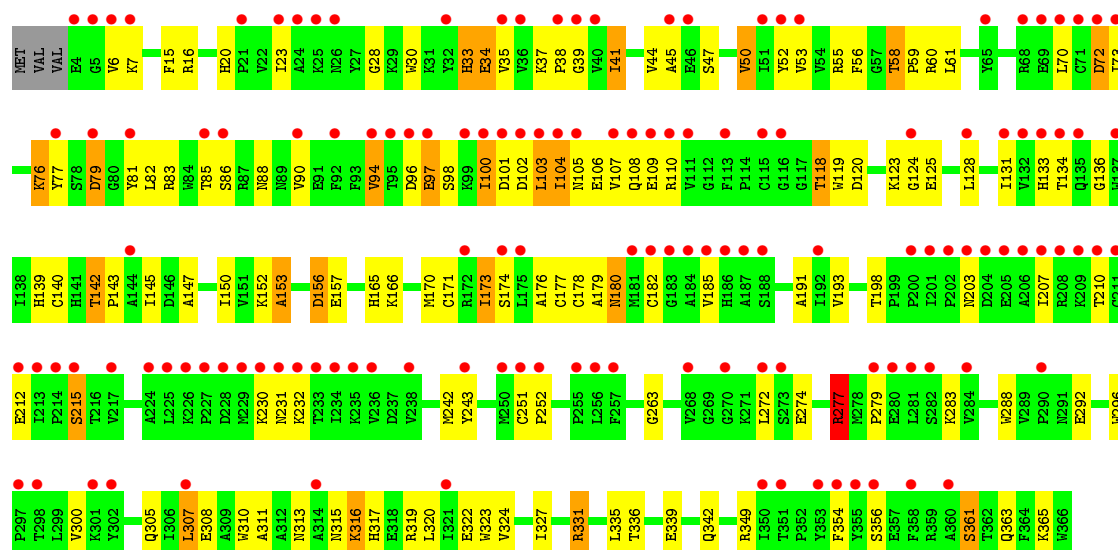


- Molecule 2: Sulfite reductase, dissimilatory-type subunit beta





- Molecule 2: Sulfite reductase, dissimilatory-type subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.84Å 69.28Å 146.33Å 90.00° 107.68° 90.00°	Depositor
Resolution (Å)	49.14 – 1.90 48.52 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.14-1.90) 98.6 (48.52-1.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.215 , 0.261 0.263 , 0.301	Depositor DCC
R_{free} test set	7014 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13292	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: CMO, SF4, SRM

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	1.29	19/3417 (0.6%)	1.05	11/4610 (0.2%)
1	D	0.64	0/3417	0.67	0/4610
2	B	1.27	12/2984 (0.4%)	1.09	11/4058 (0.3%)
2	E	0.90	8/2984 (0.3%)	0.86	3/4058 (0.1%)
All	All	1.06	39/12802 (0.3%)	0.93	25/17336 (0.1%)

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	2
2	B	0	1
All	All	0	3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	72	ASP	CB-CG	15.46	1.84	1.51
1	A	219	CYS	CB-SG	-11.10	1.63	1.82
1	A	270	ALA	CA-CB	10.18	1.73	1.52
2	E	79	ASP	C-N	9.04	1.49	1.33
1	A	266	CYS	CB-SG	8.44	1.96	1.82
2	B	274	GLU	C-O	8.28	1.39	1.23
2	B	55	ARG	CG-CD	8.19	1.72	1.51
1	A	113	ARG	C-O	7.93	1.38	1.23
1	A	284	GLU	CB-CG	7.83	1.67	1.52
1	A	263	VAL	CB-CG1	-7.74	1.36	1.52
1	A	149	CYS	CB-SG	7.67	1.95	1.82
2	B	85	THR	N-CA	7.46	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	TYR	CD2-CE2	7.43	1.50	1.39
2	B	140	CYS	CB-SG	-6.85	1.70	1.82
2	B	119	TRP	CB-CG	6.79	1.62	1.50
2	E	98	SER	CA-CB	6.78	1.63	1.52
2	B	55	ARG	CB-CG	6.74	1.70	1.52
1	A	124	SER	CB-OG	6.71	1.50	1.42
1	A	111	ALA	CA-CB	6.57	1.66	1.52
1	A	287	ARG	CZ-NH1	6.47	1.41	1.33
2	B	87	ARG	CB-CG	6.46	1.70	1.52
1	A	225	ALA	CA-CB	6.39	1.65	1.52
1	A	223	CYS	C-O	6.31	1.35	1.23
1	A	223	CYS	CB-SG	6.30	1.93	1.82
1	A	177	GLY	N-CA	-6.20	1.36	1.46
2	E	79	ASP	CG-OD2	6.02	1.39	1.25
2	E	98	SER	C-O	-5.74	1.12	1.23
1	A	285	CYS	N-CA	5.68	1.57	1.46
1	A	326	VAL	CA-CB	5.53	1.66	1.54
2	E	72	ASP	CG-OD1	-5.53	1.12	1.25
2	E	76	LYS	CD-CE	5.48	1.65	1.51
1	A	289	MET	CB-CG	5.38	1.68	1.51
1	A	107	TYR	CE1-CZ	-5.34	1.31	1.38
2	B	177	CYS	CB-SG	-5.24	1.73	1.81
2	B	185	VAL	CB-CG2	5.19	1.63	1.52
2	B	126	TYR	CB-CG	5.17	1.59	1.51
2	B	84	TRP	CE3-CZ3	5.12	1.47	1.38
2	B	84	TRP	CB-CG	5.07	1.59	1.50
2	E	331	ARG	N-CA	5.04	1.56	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	ARG	NE-CZ-NH2	-11.51	114.55	120.30
2	B	55	ARG	CG-CD-NE	-8.04	94.91	111.80
2	B	276	ARG	NE-CZ-NH1	-7.91	116.35	120.30
2	B	55	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	287	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	156	LEU	CA-CB-CG	6.43	130.08	115.30
2	E	72	ASP	CB-CG-OD2	6.04	123.73	118.30
2	B	87	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	30	LYS	CD-CE-NZ	-5.86	98.23	111.70
1	A	289	MET	N-CA-C	5.82	126.71	111.00
1	A	139	LEU	CA-CB-CG	5.72	128.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	GLY	C-N-CA	-5.70	107.45	121.70
1	A	310	LEU	CA-CB-CG	5.64	128.27	115.30
2	E	277	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	241	ASP	CB-CG-OD1	-5.55	113.31	118.30
2	B	87	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	B	57	GLY	N-CA-C	-5.41	99.57	113.10
1	A	245	ASP	CB-CG-OD1	5.26	123.03	118.30
2	B	156	ASP	CB-CG-OD2	5.25	123.03	118.30
2	B	365	LYS	CD-CE-NZ	-5.23	99.67	111.70
2	B	43	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	266	CYS	CA-CB-SG	5.08	123.14	114.00
1	A	142	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	E	72	ASP	OD1-CG-OD2	-5.01	113.77	123.30
2	B	164	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	ILE	Peptide
1	A	288	CYS	Mainchain
2	B	88	ASN	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	3330	0	3276	66	0
1	D	3330	0	3277	50	0
2	B	2901	0	2838	48	0
2	E	2901	0	2840	116	0
3	A	63	0	34	10	0
3	B	63	0	34	9	0
3	D	63	0	34	12	0
3	E	63	0	34	10	0
4	A	16	0	0	2	0
4	B	16	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	16	0	0	1	0
4	E	16	0	0	6	0
5	A	2	0	0	1	0
6	A	226	0	0	14	0
6	B	209	0	0	9	0
6	D	56	0	0	1	0
6	E	21	0	0	8	0
All	All	13292	0	12367	273	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 (273) 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)
2:E:72:ASP:CB	2:E:72:ASP:CG	1.84	1.46
2:E:134:THR:HG21	2:E:182:CYS:HB2	1.15	1.12
3:E:570:SRM:HBD2	3:E:570:SRM:HDD2	1.37	1.04
2:E:230:LYS:CB	2:E:231:ASN:HB2	1.89	1.02
1:A:219:CYS:SG	6:A:522:HOH:O	2.17	1.02
3:A:580:SRM:O1A	2:B:139:HIS:HD2	1.41	1.01
2:E:230:LYS:HB2	2:E:231:ASN:HB2	1.41	1.00
1:A:197:MET:SD	6:B:567:HOH:O	2.23	0.97
2:B:11:GLY:HA3	6:B:567:HOH:O	1.67	0.95
3:D:580:SRM:HMB1	3:D:580:SRM:HBB2	1.51	0.93
2:E:134:THR:HG21	2:E:182:CYS:CB	2.00	0.92
2:E:134:THR:CG2	2:E:182:CYS:HB2	1.99	0.92
1:A:289:MET:SD	6:A:522:HOH:O	2.28	0.91
1:A:266:CYS:SG	1:A:270:ALA:N	2.44	0.91
1:A:290:HIS:HB2	2:B:275:ALA:HB1	1.53	0.90
1:A:288:CYS:O	1:A:288:CYS:SG	2.27	0.90
1:A:379:ARG:HH11	1:A:379:ARG:HG3	1.35	0.89
3:D:580:SRM:CMB	3:D:580:SRM:HBB2	2.03	0.88
2:B:275:ALA:O	2:B:276:ARG:HB2	1.71	0.86
2:E:123:LYS:HG3	2:E:123:LYS:O	1.73	0.86
2:E:177:CYS:HB2	4:E:585:SF4:S3	2.17	0.85
2:E:124:GLY:HA3	2:E:316:LYS:HD2	1.61	0.82
1:D:379:ARG:HH11	1:D:379:ARG:HG3	1.46	0.80
3:A:580:SRM:O1A	2:B:139:HIS:CD2	2.32	0.80
1:D:128:ASN:HB2	1:D:137:ILE:HB	1.64	0.79
1:A:289:MET:CE	6:A:522:HOH:O	2.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:LYS:NZ	3:D:580:SRM:HDD2	1.98	0.78
2:E:131:ILE:HG12	2:E:173:ILE:HB	1.66	0.77
2:E:55:ARG:HH22	3:E:570:SRM:HBA2	1.49	0.77
2:E:60:ARG:HD3	2:E:133:HIS:CE1	2.21	0.76
2:E:140:CYS:SG	4:E:585:SF4:S3	2.83	0.74
1:A:262:VAL:O	1:A:263:VAL:C	2.26	0.71
1:D:398:GLU:HB2	1:D:401:GLU:HG3	1.73	0.70
2:E:263:GLY:HA3	2:E:288:TRP:NE1	2.07	0.70
2:E:94:VAL:HG12	2:E:96:ASP:H	1.55	0.70
1:A:94:PHE:O	2:B:139:HIS:HE1	1.74	0.70
1:A:229:ARG:NH1	6:A:594:HOH:O	1.92	0.70
2:E:41:ILE:HG13	2:E:53:VAL:O	1.91	0.70
1:A:5:LEU:HD11	1:A:56:LYS:HE2	1.74	0.69
2:E:313:ASN:HB3	6:E:378:HOH:O	1.92	0.69
1:A:80:ARG:NH2	3:A:580:SRM:O2A	2.21	0.69
1:A:120:GLU:HB2	2:B:64:ILE:CD1	2.23	0.68
2:B:20:HIS:HB3	2:B:23:ILE:HD12	1.76	0.67
1:A:225:ALA:O	1:A:229:ARG:HG2	1.94	0.67
1:A:379:ARG:HH11	1:A:379:ARG:CG	2.08	0.67
2:E:134:THR:HB	4:E:585:SF4:S4	2.35	0.66
2:E:323:TRP:CE2	2:E:327:ILE:HD13	2.31	0.66
1:D:379:ARG:HH11	1:D:379:ARG:CG	2.09	0.66
1:A:220:PRO:HD3	1:A:236:GLY:O	1.97	0.65
3:B:570:SRM:CBA	3:B:570:SRM:HMA3	2.14	0.65
1:D:211:LYS:HZ1	3:D:580:SRM:HDD2	1.60	0.65
1:A:371:ARG:HD3	6:E:372:HOH:O	1.96	0.64
2:E:109:GLU:N	6:E:498:HOH:O	2.30	0.64
2:E:142:THR:N	2:E:143:PRO:CD	2.61	0.64
3:E:570:SRM:CBD	3:E:570:SRM:HDD2	2.22	0.63
1:A:284:GLU:HG3	6:A:629:HOH:O	1.99	0.63
1:D:78:ILE:HG21	3:D:580:SRM:HBA1	1.81	0.62
2:E:274:GLU:HB3	2:E:363:GLN:HE21	1.64	0.62
3:A:580:SRM:C4C	2:B:182:CYS:HA	2.28	0.62
1:D:14:TRP:CD2	1:D:15:PRO:HD2	2.34	0.62
2:E:182:CYS:HG	4:E:585:SF4:FE3	1.15	0.62
1:D:243:LYS:HE3	1:D:300:LYS:HE3	1.81	0.61
2:E:37:LYS:HB2	2:E:38:PRO:HD2	1.82	0.61
2:E:107:VAL:C	6:E:498:HOH:O	2.38	0.61
2:B:170:MET:SD	3:B:570:SRM:HBD1	2.41	0.61
2:E:263:GLY:HA3	2:E:288:TRP:CD1	2.36	0.61
2:E:52:TYR:CE1	2:E:97:GLU:HB3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ALA:HB3	4:A:576:SF4:S3	2.40	0.60
2:B:274:GLU:OE1	2:B:363:GLN:HG3	2.02	0.60
1:D:15:PRO:HB2	2:E:59:PRO:HG3	1.82	0.60
2:B:242:MET:SD	2:B:244:CYS:HB3	2.42	0.60
1:A:288:CYS:O	2:B:275:ALA:HA	2.02	0.59
2:E:56:PHE:CE2	2:E:107:VAL:HG11	2.37	0.59
1:A:289:MET:HE1	6:A:522:HOH:O	1.97	0.59
2:E:44:VAL:HG22	2:E:50:VAL:HG22	1.85	0.59
2:E:52:TYR:HE1	2:E:97:GLU:HB3	1.66	0.59
2:B:134:THR:OG1	2:B:177:CYS:SG	2.34	0.59
2:E:176:ALA:HB2	2:E:185:VAL:HG21	1.85	0.59
2:E:123:LYS:O	2:E:123:LYS:CG	2.47	0.59
2:E:58:THR:HG22	2:E:90:VAL:HG12	1.85	0.59
1:D:315:ALA:HB1	1:D:316:PRO:CD	2.33	0.58
2:E:182:CYS:SG	4:E:585:SF4:S2	2.97	0.58
2:B:330:GLU:O	2:B:334:GLU:HG3	2.02	0.58
1:A:417:TRP:CD1	1:A:417:TRP:C	2.76	0.58
2:E:305:GLN:NE2	2:E:336:THR:O	2.34	0.58
1:A:94:PHE:O	2:B:139:HIS:CE1	2.56	0.58
2:B:276:ARG:HG3	2:B:276:ARG:NH1	2.18	0.57
2:E:272:LEU:HB2	3:E:570:SRM:CCC	2.34	0.57
1:D:128:ASN:ND2	2:E:61:LEU:HD12	2.19	0.57
2:E:33:HIS:CD2	2:E:34:GLU:N	2.72	0.57
2:B:170:MET:CE	3:B:570:SRM:HBD1	2.34	0.57
2:E:86:SER:OG	3:E:570:SRM:HAB1	2.04	0.57
3:B:570:SRM:C1A	3:B:570:SRM:HBA1	2.35	0.57
1:A:14:TRP:CD2	1:A:15:PRO:HD2	2.41	0.56
2:E:76:LYS:HD3	2:E:77:TYR:CE1	2.40	0.56
2:E:185:VAL:HG11	2:E:193:VAL:HG22	1.87	0.56
1:A:186:TYR:OH	1:A:216:CYS:HB3	2.05	0.56
1:D:151:GLU:HG2	2:E:6:VAL:HG22	1.87	0.56
2:E:323:TRP:NE1	2:E:327:ILE:HD13	2.21	0.56
3:D:580:SRM:HMB1	3:D:580:SRM:CBB	2.32	0.56
2:E:145:ILE:HB	2:E:150:ILE:HD11	1.87	0.56
2:E:97:GLU:O	2:E:100:ILE:HD11	2.06	0.56
1:D:96:THR:HG23	2:E:139:HIS:CE1	2.41	0.55
2:B:366:TRP:CE3	2:B:366:TRP:HA	2.40	0.55
2:B:320:LEU:N	6:B:489:HOH:O	2.32	0.55
1:A:223:CYS:HB3	3:B:570:SRM:C4B	2.37	0.55
2:B:134:THR:HB	4:B:585:SF4:S4	2.46	0.55
2:E:108:GLN:N	6:E:498:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:157:GLU:HG3	2:E:300:VAL:HG11	1.87	0.55
1:D:128:ASN:HD22	2:E:61:LEU:HA	1.72	0.55
1:D:147:GLN:HB3	1:D:148:PRO:HD3	1.89	0.55
1:D:178:PRO:HG3	1:D:187:ASP:HA	1.89	0.54
1:A:170:ARG:HH12	5:A:590:CMO:C	2.20	0.54
2:E:279:PRO:HD2	2:E:361:SER:HB2	1.88	0.54
2:B:11:GLY:CA	6:B:567:HOH:O	2.38	0.54
1:A:99:ILE:HD13	1:A:99:ILE:N	2.22	0.54
1:A:69:SER:HB2	6:A:544:HOH:O	2.08	0.54
2:E:153:ALA:O	2:E:156:ASP:HB2	2.07	0.53
3:A:580:SRM:CBB	3:A:580:SRM:CMB	2.87	0.53
2:B:11:GLY:N	6:B:567:HOH:O	2.40	0.53
1:D:211:LYS:HZ2	3:D:580:SRM:HDD2	1.70	0.53
1:A:98:ARG:C	1:A:99:ILE:HD13	2.28	0.53
2:B:147:ALA:HB2	2:B:177:CYS:SG	2.49	0.53
2:E:56:PHE:CD2	2:E:107:VAL:HG11	2.44	0.53
3:A:580:SRM:HHB	3:A:580:SRM:HBA1	1.90	0.52
1:D:399:LYS:HD3	1:D:417:TRP:O	2.10	0.52
1:A:223:CYS:HB3	3:B:570:SRM:CHC	2.39	0.52
1:A:379:ARG:NH1	1:A:379:ARG:HG3	2.15	0.52
1:A:56:LYS:NZ	6:A:546:HOH:O	2.23	0.52
2:B:275:ALA:O	2:B:276:ARG:CB	2.44	0.52
1:A:289:MET:HG3	6:A:522:HOH:O	2.10	0.51
2:E:6:VAL:HG12	2:E:7:LYS:O	2.11	0.51
1:D:151:GLU:HG2	2:E:6:VAL:CG2	2.40	0.51
1:D:288:CYS:O	1:D:289:MET:HB2	2.11	0.51
2:E:210:THR:HG21	2:E:252:PRO:HG3	1.93	0.51
2:E:39:GLY:N	2:E:118:THR:OG1	2.37	0.51
1:A:96:THR:HG23	2:B:139:HIS:NE2	2.25	0.51
1:D:186:TYR:CD1	1:D:333:VAL:HG11	2.46	0.51
2:E:320:LEU:O	2:E:324:VAL:HG23	2.10	0.51
1:A:289:MET:CG	6:A:522:HOH:O	2.57	0.50
2:E:106:GLU:C	6:E:498:HOH:O	2.48	0.50
2:E:170:MET:O	2:E:319:ARG:HG2	2.11	0.50
2:B:177:CYS:HB2	4:B:585:SF4:S3	2.51	0.50
3:D:580:SRM:CMB	3:D:580:SRM:CBB	2.78	0.50
1:A:56:LYS:CE	6:A:546:HOH:O	2.57	0.50
1:A:300:LYS:HD3	6:B:571:HOH:O	2.10	0.50
2:E:110:ARG:N	6:E:498:HOH:O	2.28	0.50
1:D:338:ASP:O	1:D:342:GLU:HB2	2.12	0.50
1:A:257:ASP:O	1:A:261:GLU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:263:GLY:HA3	2:E:288:TRP:HE1	1.74	0.49
1:D:387:LYS:HE3	2:E:356:SER:O	2.12	0.49
3:A:580:SRM:C1C	2:B:182:CYS:HA	2.42	0.49
1:D:179:ALA:O	2:E:30:TRP:HZ2	1.96	0.49
2:E:103:LEU:O	2:E:106:GLU:N	2.45	0.49
2:E:230:LYS:CA	2:E:231:ASN:HB2	2.42	0.49
1:D:128:ASN:HD21	2:E:61:LEU:HD12	1.78	0.49
3:D:580:SRM:HBD1	3:D:580:SRM:HHD	1.94	0.49
3:D:580:SRM:HMB3	3:D:580:SRM:HBB2	1.93	0.49
2:B:134:THR:HG21	2:B:182:CYS:HB2	1.95	0.49
2:B:276:ARG:HH11	2:B:276:ARG:HG3	1.78	0.48
1:A:223:CYS:HA	3:B:570:SRM:C1C	2.44	0.48
1:A:382:ASP:O	1:A:385:MET:HG3	2.14	0.48
3:A:580:SRM:NC	2:B:182:CYS:HA	2.28	0.48
2:E:125:GLU:HB3	2:E:165:HIS:HB3	1.96	0.48
1:A:147:GLN:HB3	1:A:148:PRO:HD3	1.95	0.48
2:B:342:GLN:HG2	1:D:371:ARG:HG3	1.96	0.48
2:E:30:TRP:HA	2:E:45:ALA:HA	1.95	0.48
2:E:44:VAL:HG22	2:E:50:VAL:CG2	2.44	0.47
1:D:273:TRP:HB2	1:D:278:LEU:HD12	1.97	0.47
1:A:219:CYS:HB2	6:A:522:HOH:O	2.12	0.47
1:A:132:SER:O	1:A:229:ARG:NH2	2.48	0.47
2:E:20:HIS:HA	2:E:81:TYR:CD1	2.49	0.47
1:D:119:TRP:CH2	1:D:141:THR:HB	2.50	0.47
2:E:131:ILE:HG23	2:E:174:SER:HA	1.97	0.46
2:E:85:THR:HB	3:E:570:SRM:HAB2	1.98	0.46
3:B:570:SRM:HMB2	3:B:570:SRM:HBB	1.50	0.46
2:B:134:THR:CG2	2:B:182:CYS:HB2	2.45	0.46
2:E:97:GLU:O	2:E:100:ILE:CD1	2.63	0.46
2:E:185:VAL:HG13	2:E:191:ALA:HB1	1.96	0.46
2:E:136:GLY:N	2:E:177:CYS:SG	2.89	0.46
1:A:120:GLU:HB2	2:B:64:ILE:HD11	1.97	0.46
1:A:197:MET:CE	6:B:567:HOH:O	2.57	0.46
2:E:307:LEU:HD23	2:E:308:GLU:N	2.31	0.46
2:B:64:ILE:HD13	2:B:64:ILE:HG21	1.70	0.45
2:E:15:PHE:CG	2:E:16:ARG:N	2.84	0.45
2:E:72:ASP:CG	2:E:72:ASP:CA	2.76	0.45
2:B:138:ILE:HG13	6:B:379:HOH:O	2.15	0.45
1:A:81:TYR:HE2	1:A:93:HIS:CE1	2.34	0.45
3:E:570:SRM:HHA	3:E:570:SRM:HMA2	1.72	0.45
1:A:241:ASP:N	1:A:241:ASP:OD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:ALA:HB3	1:D:229:ARG:HD3	1.97	0.45
1:D:50:GLN:HE21	1:D:50:GLN:HB2	1.60	0.45
2:E:55:ARG:NH2	3:E:570:SRM:HBA2	2.25	0.45
1:A:326:VAL:HB	1:A:385:MET:HA	1.98	0.45
2:E:134:THR:CG2	2:E:182:CYS:CB	2.77	0.45
2:E:277:ARG:HG2	2:E:322:GLU:HG2	1.99	0.45
1:D:131:GLY:HA3	3:D:580:SRM:HBB1	1.99	0.45
2:E:310:TRP:O	2:E:311:ALA:C	2.55	0.44
1:A:169:LEU:O	1:A:203:LEU:HA	2.17	0.44
2:E:292:GLU:HB2	2:E:296:TRP:HA	1.99	0.44
1:A:379:ARG:NH1	1:A:379:ARG:CG	2.72	0.44
2:E:142:THR:N	2:E:143:PRO:HD3	2.33	0.44
1:A:25:ALA:O	1:A:29:GLU:HB2	2.17	0.44
1:D:379:ARG:NH1	1:D:379:ARG:CG	2.73	0.44
2:B:346:ASP:HB3	2:E:354:PHE:HB2	1.99	0.44
1:D:218:GLY:HA3	4:D:575:SF4:S2	2.58	0.44
1:D:65:GLY:HA2	1:D:81:TYR:CD1	2.53	0.44
2:E:103:LEU:O	2:E:104:ILE:C	2.56	0.44
1:D:222:ASP:OD1	1:D:227:LYS:HG2	2.18	0.44
1:A:39:LYS:HG2	1:A:121:LYS:O	2.18	0.44
2:B:322:GLU:OE1	6:B:420:HOH:O	2.21	0.43
2:E:73:ILE:HD11	2:E:110:ARG:HD3	2.00	0.43
2:E:315:ASN:O	2:E:316:LYS:C	2.56	0.43
2:E:33:HIS:HD2	2:E:34:GLU:N	2.16	0.43
1:A:220:PRO:HG2	1:A:287:ARG:O	2.18	0.43
1:D:142:ARG:HB2	1:D:145:TYR:CD2	2.54	0.43
1:D:153:LEU:HD23	1:D:153:LEU:HA	1.88	0.43
1:D:387:LYS:HB2	1:D:387:LYS:HE2	1.79	0.43
2:E:230:LYS:HE3	2:E:231:ASN:OD1	2.19	0.43
1:D:317:PHE:HA	1:D:318:VAL:HA	1.73	0.43
1:D:110:LYS:HD2	1:D:158:ILE:HD12	2.00	0.43
1:D:178:PRO:O	2:E:28:GLY:N	2.48	0.43
1:D:257:ASP:OD2	1:D:260:ASN:HB2	2.18	0.43
2:E:58:THR:C	2:E:60:ARG:H	2.22	0.43
2:E:86:SER:H	3:E:570:SRM:HAB1	1.84	0.43
1:A:315:ALA:HB1	1:A:316:PRO:HD2	2.01	0.43
1:A:81:TYR:CE2	1:A:93:HIS:ND1	2.87	0.43
2:E:339:GLU:HG2	6:E:381:HOH:O	2.18	0.43
2:B:175:LEU:C	2:B:175:LEU:HD23	2.39	0.42
2:E:37:LYS:HB2	2:E:38:PRO:CD	2.49	0.42
2:E:212:GLU:HB3	2:E:215:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASN:HA	6:A:511:HOH:O	2.19	0.42
2:B:126:TYR:OH	2:B:317:HIS:ND1	2.50	0.42
2:B:197:ARG:HD3	2:B:288:TRP:CD1	2.54	0.42
3:A:580:SRM:C3C	2:B:182:CYS:HA	2.50	0.42
1:D:174:ALA:HB1	1:D:188:THR:HB	2.02	0.42
2:B:146:ASP:O	2:B:150:ILE:HD12	2.19	0.42
3:B:570:SRM:HMA3	3:B:570:SRM:HBA1	2.00	0.42
2:B:366:TRP:O	2:E:331:ARG:NH2	2.53	0.42
1:A:176:MET:HG2	4:A:575:SF4:S1	2.60	0.42
1:A:37:ASP:OD2	1:A:121:LYS:HE3	2.19	0.42
2:E:133:HIS:HB2	2:E:147:ALA:HB1	2.00	0.42
2:B:137:TRP:CE3	2:B:146:ASP:HB2	2.55	0.41
2:B:90:VAL:HG22	2:B:91:GLU:N	2.35	0.41
1:D:290:HIS:N	6:D:540:HOH:O	2.36	0.41
2:E:128:LEU:HD12	2:E:171:CYS:O	2.19	0.41
2:E:58:THR:HG23	2:E:88:ASN:O	2.20	0.41
2:E:203:ASN:O	2:E:207:ILE:HG13	2.19	0.41
2:E:307:LEU:HD23	2:E:308:GLU:HG3	2.02	0.41
3:E:570:SRM:HMA3	3:E:570:SRM:HAA2	1.56	0.41
1:A:319:GLU:OE1	2:E:349:ARG:NH1	2.53	0.41
3:A:580:SRM:HMB3	3:A:580:SRM:HBB2	2.01	0.41
1:D:399:LYS:HB2	1:D:399:LYS:HE3	1.77	0.41
2:E:178:CYS:SG	2:E:180:ASN:HB2	2.61	0.41
1:A:219:CYS:CB	6:A:522:HOH:O	2.52	0.41
1:A:417:TRP:HD1	1:A:417:TRP:C	2.22	0.41
1:D:128:ASN:HD21	2:E:61:LEU:CD1	2.33	0.41
1:A:394:PHE:CE2	2:E:179:ALA:HB1	2.56	0.41
1:D:284:GLU:HA	2:E:365:LYS:HE2	2.03	0.41
1:D:110:LYS:HD2	1:D:158:ILE:CD1	2.50	0.41
2:E:323:TRP:CE2	2:E:327:ILE:CD1	3.02	0.41
2:E:70:LEU:HD23	2:E:70:LEU:HA	1.83	0.41
2:E:35:VAL:HB	2:E:120:ASP:OD1	2.20	0.41
1:D:78:ILE:HG21	3:D:580:SRM:CBA	2.50	0.41
2:E:320:LEU:C	2:E:320:LEU:HD23	2.41	0.41
1:A:271:ILE:HA	1:A:279:THR:O	2.21	0.40
2:B:57:GLY:HA2	2:B:89:ASN:OD1	2.21	0.40
1:A:186:TYR:CD1	1:A:333:VAL:HG11	2.56	0.40
2:E:316:LYS:HG3	2:E:317:HIS:CD2	2.56	0.40
2:E:177:CYS:CB	4:E:585:SF4:S3	2.99	0.40
2:B:191:ALA:HB3	2:B:267:MET:HB2	2.03	0.40
2:E:342:GLN:OE1	2:E:342:GLN:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:VAL:HG21	2:E:119:TRP:O	2.22	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	415/418 (99%)	394 (95%)	19 (5%)	2 (0%)	32	20
1	D	415/418 (99%)	391 (94%)	24 (6%)	0	100	100
2	B	361/366 (99%)	339 (94%)	18 (5%)	4 (1%)	17	6
2	E	361/366 (99%)	309 (86%)	44 (12%)	8 (2%)	8	1
All	All	1552/1568 (99%)	1433 (92%)	105 (7%)	14 (1%)	20	8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	103	LEU
2	E	104	ILE
1	A	289	MET
2	E	34	GLU
2	E	79	ASP
2	E	153	ALA
2	E	232	LYS
2	B	182	CYS
1	A	290	HIS
2	B	60	ARG
2	E	156	ASP
2	B	276	ARG
2	B	142	THR
2	E	142	THR

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	353/354 (100%)	337 (96%)	16 (4%)	32	21
1	D	353/354 (100%)	343 (97%)	10 (3%)	49	40
2	B	314/317 (99%)	301 (96%)	13 (4%)	35	24
2	E	314/317 (99%)	284 (90%)	30 (10%)	10	3
All	All	1334/1342 (99%)	1265 (95%)	69 (5%)	27	16

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	MET
1	A	50	GLN
1	A	68	VAL
1	A	144	GLU
1	A	210	TYR
1	A	216	CYS
1	A	219	CYS
1	A	229	ARG
1	A	243	LYS
1	A	278	LEU
1	A	279	THR
1	A	286	VAL
1	A	288	CYS
1	A	371	ARG
1	A	383	VAL
1	A	417	TRP
2	B	4	GLU
2	B	93	PHE
2	B	97	GLU
2	B	108	GLN
2	B	177	CYS
2	B	188	SER
2	B	230	LYS
2	B	242	MET

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Mol	Chain	Res	Type
2	B	243	TYR
2	B	277	ARG
2	B	283	LYS
2	B	297	PRO
2	B	307	LEU
1	D	50	GLN
1	D	100	ASN
1	D	132	SER
1	D	133	THR
1	D	144	GLU
1	D	210	TYR
1	D	224	VAL
1	D	334	GLU
1	D	379	ARG
1	D	413	LYS
2	E	23	ILE
2	E	33	HIS
2	E	41	ILE
2	E	47	SER
2	E	50	VAL
2	E	58	THR
2	E	82	LEU
2	E	83	ARG
2	E	94	VAL
2	E	97	GLU
2	E	100	ILE
2	E	101	ASP
2	E	102	ASP
2	E	105	ASN
2	E	118	THR
2	E	152	LYS
2	E	166	LYS
2	E	173	ILE
2	E	180	ASN
2	E	198	THR
2	E	215	SER
2	E	242	MET
2	E	243	TYR
2	E	251	CYS
2	E	277	ARG
2	E	283	LYS
2	E	307	LEU

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Mol	Chain	Res	Type
2	E	316	LYS
2	E	335	LEU
2	E	361	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
2	B	139	HIS
1	D	50	GLN
1	D	100	ASN
1	D	128	ASN
1	D	282	ASN
2	E	33	HIS
2	E	180	ASN
2	E	363	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

13 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
4	SF4	A	575	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	A	576	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SRM	A	580	2	34,70,70	2.02	8 (23%)	34,112,112	3.55	12 (35%)
5	CMO	A	590	-	0,1,1	0.00	-	0,0,0	0.00	-
3	SRM	B	570	1	34,70,70	2.87	14 (41%)	34,112,112	7.40	24 (70%)
4	SF4	B	585	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	586	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	D	575	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	D	576	1,6	0,12,12	0.00	-	0,24,24	0.00	-
3	SRM	D	580	-	34,70,70	1.94	8 (23%)	34,112,112	3.50	15 (44%)
3	SRM	E	570	1	34,70,70	2.47	11 (32%)	34,112,112	3.92	22 (64%)
4	SF4	E	585	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	E	586	2	0,12,12	0.00	-	0,24,24	0.00	-

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
4	SF4	A	575	1	-	0/0/48/48	0/6/5/5
4	SF4	A	576	1	-	0/0/48/48	0/6/5/5
3	SRM	A	580	2	-	0/22/126/126	0/0/8/8
5	CMO	A	590	-	-	0/0/0/0	0/0/0/0
3	SRM	B	570	1	-	0/22/126/126	0/0/8/8
4	SF4	B	585	2	-	0/0/48/48	0/6/5/5
4	SF4	B	586	2	-	0/0/48/48	0/6/5/5
4	SF4	D	575	1	-	0/0/48/48	0/6/5/5
4	SF4	D	576	1,6	-	0/0/48/48	0/6/5/5
3	SRM	D	580	-	-	0/22/126/126	0/0/8/8
3	SRM	E	570	1	-	1/22/126/126	0/0/8/8
4	SF4	E	585	2	-	0/0/48/48	0/6/5/5
4	SF4	E	586	2	-	0/0/48/48	0/6/5/5

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	570	SRM	C4C-NC	-7.56	1.27	1.36
3	B	570	SRM	C4B-NB	-7.25	1.25	1.39
3	B	570	SRM	C1B-NB	-5.84	1.28	1.38
3	E	570	SRM	C1C-NC	-5.54	1.30	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	570	SRM	C4C-NC	-5.29	1.30	1.36
3	E	570	SRM	C4A-NA	-4.37	1.30	1.39
3	B	570	SRM	C1D-ND	-4.10	1.27	1.36
3	B	570	SRM	C4A-NA	-3.79	1.31	1.39
3	D	580	SRM	C4A-NA	-3.07	1.33	1.39
3	E	570	SRM	C1B-NB	-2.99	1.32	1.38
3	B	570	SRM	C1D-CHD	-2.88	1.32	1.40
3	A	580	SRM	C4A-NA	-2.80	1.33	1.39
3	B	570	SRM	CHC-C4B	-2.47	1.33	1.39
3	E	570	SRM	CDA-C2A	-2.45	1.52	1.56
3	B	570	SRM	C4D-ND	-2.20	1.31	1.36
3	D	580	SRM	C1A-NA	-2.14	1.34	1.38
3	D	580	SRM	C4C-NC	-2.07	1.34	1.36
3	E	570	SRM	C1A-NA	-2.07	1.34	1.38
3	A	580	SRM	CAB-C3B	2.06	1.55	1.51
3	B	570	SRM	CDD-C3D	2.07	1.57	1.52
3	E	570	SRM	CDC-C2C	2.25	1.55	1.52
3	D	580	SRM	CAD-C2D	2.26	1.55	1.52
3	E	570	SRM	CHA-C1A	2.26	1.39	1.36
3	A	580	SRM	CAD-C2D	2.52	1.56	1.52
3	A	580	SRM	CHA-C1A	2.64	1.40	1.36
3	B	570	SRM	CDA-C2A	2.74	1.60	1.56
3	B	570	SRM	C1A-NA	2.90	1.43	1.38
3	B	570	SRM	C3C-C2C	3.10	1.46	1.37
3	E	570	SRM	CAD-C2D	3.17	1.57	1.52
3	D	580	SRM	FE-NA	3.56	2.09	1.95
3	D	580	SRM	FE-NB	3.79	2.10	1.95
3	B	570	SRM	C3D-C2D	3.89	1.48	1.39
3	D	580	SRM	C3C-C2C	4.19	1.50	1.37
3	A	580	SRM	FE-NB	4.23	2.12	1.95
3	A	580	SRM	FE-NA	4.55	2.13	1.95
3	B	570	SRM	CHB-C4A	4.59	1.49	1.39
3	A	580	SRM	C3C-C2C	4.60	1.51	1.37
3	E	570	SRM	C3C-C2C	5.06	1.52	1.37
3	A	580	SRM	C3D-C2D	6.16	1.54	1.39
3	D	580	SRM	C3D-C2D	6.32	1.54	1.39
3	E	570	SRM	C3D-C2D	6.66	1.55	1.39

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	SRM	CAA-C3A-C2A	-19.87	101.06	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	SRM	CAB-C3B-C2B	-17.18	104.10	123.52
3	B	570	SRM	C4A-NA-C1A	-15.61	95.85	106.37
3	A	580	SRM	CAB-C3B-C2B	-15.01	106.55	123.52
3	E	570	SRM	CAA-C3A-C2A	-13.00	108.83	123.52
3	D	580	SRM	CDD-C3D-C4D	-11.60	109.78	127.36
3	B	570	SRM	C3B-C4B-NB	-9.92	98.78	110.12
3	D	580	SRM	CAB-C3B-C2B	-6.84	115.79	123.52
3	D	580	SRM	CDD-C3D-C2D	-6.39	114.95	126.48
3	B	570	SRM	C3B-C2B-C1B	-6.37	89.96	101.25
3	B	570	SRM	CEC-CDC-C2C	-6.11	104.24	116.14
3	E	570	SRM	C4A-NA-C1A	-5.81	102.45	106.37
3	E	570	SRM	CDC-C2C-C3C	-5.64	116.31	126.48
3	B	570	SRM	CHA-C1A-NA	-5.62	115.33	124.18
3	D	580	SRM	CAD-C2D-C3D	-5.49	115.71	129.38
3	A	580	SRM	CDD-C3D-C2D	-4.95	117.55	126.48
3	E	570	SRM	CDC-C2C-C1C	-4.59	120.46	127.39
3	D	580	SRM	CAA-C3A-C2A	-4.48	118.45	123.52
3	B	570	SRM	CAC-CBC-CCC	-4.44	105.07	112.66
3	E	570	SRM	C4D-CHA-C1A	-4.37	121.47	130.12
3	E	570	SRM	CEC-CDC-C2C	-4.24	107.88	116.14
3	A	580	SRM	CAA-C3A-C2A	-4.12	118.86	123.52
3	E	570	SRM	CBC-CAC-C3C	-4.09	104.66	112.47
3	B	570	SRM	CBC-CAC-C3C	-3.90	105.02	112.47
3	E	570	SRM	C3B-C2B-C1B	-3.77	94.58	101.25
3	E	570	SRM	CAC-C3C-C2C	-3.72	120.11	129.38
3	A	580	SRM	C3A-C2A-C1A	-3.67	94.75	101.25
3	E	570	SRM	CHB-C4A-C3A	-3.64	117.21	125.47
3	D	580	SRM	C3A-C2A-C1A	-3.58	94.90	101.25
3	B	570	SRM	CHB-C4A-C3A	-3.58	117.35	125.47
3	B	570	SRM	C3A-C2A-C1A	-3.25	95.50	101.25
3	D	580	SRM	C3A-C4A-NA	-3.06	106.63	110.12
3	E	570	SRM	CAB-C3B-C2B	-2.99	120.15	123.52
3	B	570	SRM	C2B-C1B-CHB	-2.88	113.96	124.10
3	E	570	SRM	CDD-C3D-C2D	-2.86	121.33	126.48
3	D	580	SRM	CAA-CBA-CCA	-2.78	107.91	112.66
3	D	580	SRM	C3B-C2B-C1B	-2.66	96.54	101.25
3	A	580	SRM	CAC-CBC-CCC	-2.65	108.13	112.66
3	E	570	SRM	C2B-C1B-CHB	-2.53	115.19	124.10
3	B	570	SRM	CDD-C3D-C2D	-2.37	122.21	126.48
3	A	580	SRM	CAD-C2D-C3D	-2.36	123.52	129.38
3	D	580	SRM	C4D-CHA-C1A	-2.34	125.47	130.12
3	E	570	SRM	CDD-C3D-C4D	-2.31	123.86	127.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	580	SRM	C3B-C2B-C1B	-2.28	97.22	101.25
3	D	580	SRM	CHA-C1A-NA	-2.25	120.64	124.18
3	E	570	SRM	C2A-C1A-CHA	-2.05	116.88	124.10
3	E	570	SRM	C2A-CDA-CEA	2.04	118.41	115.39
3	B	570	SRM	C4D-CHA-C1A	2.12	134.31	130.12
3	D	580	SRM	CDC-C2C-C1C	2.16	130.66	127.39
3	E	570	SRM	CAB-CBB-CCB	2.20	116.42	112.66
3	B	570	SRM	CAB-CBB-CCB	2.45	116.84	112.66
3	A	580	SRM	C3B-C4B-NB	2.53	113.01	110.12
3	A	580	SRM	CDC-C2C-C1C	2.59	131.30	127.39
3	E	570	SRM	CAA-CBA-CCA	2.61	117.12	112.66
3	D	580	SRM	C3B-C4B-NB	2.71	113.21	110.12
3	E	570	SRM	CED-CDD-C3D	3.37	122.71	116.14
3	B	570	SRM	C2A-CDA-CEA	3.40	120.42	115.39
3	E	570	SRM	C2B-CDB-CEB	3.55	120.65	115.39
3	B	570	SRM	C1C-CHC-C4B	3.63	138.47	124.02
3	B	570	SRM	CDD-C3D-C4D	3.71	133.00	127.36
3	D	580	SRM	CBD-CAD-C2D	4.14	120.39	112.48
3	B	570	SRM	CDC-C2C-C1C	4.42	134.07	127.39
3	A	580	SRM	C4A-NA-C1A	4.45	109.37	106.37
3	B	570	SRM	CHC-C4B-NB	5.16	133.49	123.80
3	B	570	SRM	CHB-C1B-NB	5.73	133.20	124.18
3	A	580	SRM	C2A-CDA-CEA	6.03	124.32	115.39
3	E	570	SRM	CBD-CAD-C2D	6.08	124.12	112.48
3	A	580	SRM	CBD-CAD-C2D	6.34	124.60	112.48
3	E	570	SRM	C3A-C4A-NA	6.96	118.08	110.12
3	D	580	SRM	C4A-NA-C1A	7.11	111.16	106.37
3	B	570	SRM	CBD-CAD-C2D	9.19	130.05	112.48
3	B	570	SRM	C3A-C4A-NA	10.42	122.03	110.12
3	B	570	SRM	C4B-NB-C1B	17.51	118.17	106.37

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	570	SRM	C3D-C2D-CAD-CBD

There are no ring outliers.

10 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	575	SF4	1	0
4	A	576	SF4	1	0
3	A	580	SRM	10	0
5	A	590	CMO	1	0
3	B	570	SRM	9	0
4	B	585	SF4	2	0
4	D	575	SF4	1	0
3	D	580	SRM	12	0
3	E	570	SRM	10	0
4	E	585	SF4	6	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	417/418 (99%)	0.73	49 (11%) 5 5	4, 17, 30, 66	0
1	D	417/418 (99%)	1.53	116 (27%) 1 0	7, 15, 28, 38	0
2	B	363/366 (99%)	0.78	44 (12%) 5 5	8, 17, 26, 51	0
2	E	363/366 (99%)	1.81	137 (37%) 0 0	2, 12, 36, 55	0
All	All	1560/1568 (99%)	1.21	346 (22%) 1 1	2, 16, 30, 66	0

All (346) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	229	MET	9.8
1	D	81	TYR	8.6
2	E	4	GLU	8.5
1	D	67	ILE	8.1
2	E	184	ALA	7.9
1	D	33	ALA	7.5
1	D	91	VAL	7.5
1	D	25	ALA	7.2
2	E	234	ILE	6.8
2	E	183	GLY	6.8
1	D	32	ALA	6.6
2	E	5	GLY	6.6
1	D	88	ILE	6.6
2	E	206	ALA	6.4
2	E	100	ILE	6.3
1	D	30	LYS	5.8
1	D	31	ALA	5.7
1	D	1	SER	5.7
1	D	276	LYS	5.6
2	E	233	THR	5.5
2	E	207	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	406	ALA	5.4
1	A	416	MET	5.4
1	D	5	LEU	5.3
1	D	94	PHE	5.2
2	E	6	VAL	5.2
2	E	40	VAL	5.2
2	E	77	TYR	5.2
2	E	232	LYS	5.2
1	A	417	TRP	5.1
2	E	185	VAL	5.0
2	E	35	VAL	4.9
2	E	51	ILE	4.9
2	E	109	GLU	4.8
2	E	111	VAL	4.8
2	E	201	ILE	4.8
2	E	209	LYS	4.8
2	B	5	GLY	4.8
1	D	228	ALA	4.7
2	E	187	ALA	4.7
2	E	95	THR	4.5
2	B	272	LEU	4.5
2	E	225	LEU	4.4
1	D	157	GLU	4.4
2	E	205	GLU	4.4
1	D	158	ILE	4.4
1	D	132	SER	4.4
2	E	236	VAL	4.4
2	E	355	TYR	4.4
1	D	255	TRP	4.4
2	B	4	GLU	4.3
1	D	315	ALA	4.2
1	D	40	MET	4.1
1	D	86	GLU	4.1
1	D	229	ARG	4.1
2	E	25	LYS	4.1
2	E	281	LEU	4.1
2	E	211	CYS	4.1
1	D	42	LYS	4.1
2	B	355	TYR	4.0
2	E	182	CYS	4.0
2	B	353	TYR	4.0
1	A	313	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	273	TRP	3.9
2	E	69	GLU	3.9
1	A	407	TYR	3.9
1	A	273	TRP	3.9
2	E	132	VAL	3.9
1	D	45	ARG	3.9
2	E	256	LEU	3.9
1	D	65	GLY	3.9
2	B	175	LEU	3.9
2	E	97	GLU	3.9
2	E	210	THR	3.9
2	E	115	CYS	3.9
2	E	213	ILE	3.9
1	D	131	GLY	3.9
2	E	124	GLY	3.9
1	D	43	GLY	3.8
2	E	251	CYS	3.8
1	D	24	THR	3.8
1	A	404	PRO	3.8
2	E	53	VAL	3.8
2	E	302	TYR	3.8
1	D	145	TYR	3.7
2	E	71	CYS	3.7
1	A	228	ALA	3.7
2	E	230	LYS	3.7
2	E	188	SER	3.7
1	A	279	THR	3.7
1	D	332	GLU	3.7
2	E	96	ASP	3.7
1	D	27	LEU	3.6
1	D	323	ILE	3.6
1	A	106	PHE	3.6
2	E	90	VAL	3.6
2	E	21	PRO	3.6
1	D	59	LYS	3.6
2	E	110	ARG	3.6
2	E	104	ILE	3.5
1	A	276	LYS	3.5
2	E	32	TYR	3.5
2	E	107	VAL	3.5
2	E	226	LYS	3.4
2	E	208	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	214	PRO	3.4
1	D	321	ALA	3.4
2	E	200	PRO	3.4
1	D	68	VAL	3.4
2	E	94	VAL	3.4
2	E	353	TYR	3.4
1	D	144	GLU	3.4
1	D	89	PRO	3.4
1	D	71	VAL	3.4
1	D	247	GLU	3.3
1	D	134	GLY	3.3
1	D	69	SER	3.3
1	D	417	TRP	3.3
2	E	92	PHE	3.3
1	A	411	LEU	3.3
2	E	65	TYR	3.3
1	D	272	LYS	3.3
1	D	313	GLY	3.3
2	E	45	ALA	3.3
2	E	255	PRO	3.3
1	D	227	LYS	3.3
2	E	72	ASP	3.3
2	E	73	ILE	3.3
1	D	320	GLY	3.3
2	E	227	PRO	3.3
1	D	87	GLN	3.3
2	B	281	LEU	3.3
1	D	154	GLY	3.2
1	D	275	GLY	3.2
2	E	186	HIS	3.2
2	E	81	TYR	3.2
2	E	68	ARG	3.2
2	E	26	ASN	3.2
1	D	244	VAL	3.2
1	A	405	SER	3.2
1	A	322	VAL	3.2
2	E	52	TYR	3.2
2	E	137	TRP	3.1
2	B	187	ALA	3.1
1	D	36	LYS	3.1
1	A	414	ARG	3.1
1	D	115	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	358	PHE	3.1
2	E	282	SER	3.1
2	E	46	GLU	3.1
2	E	231	ASN	3.1
1	D	366	TRP	3.1
2	B	174	SER	3.1
1	A	323	ILE	3.1
2	E	181	MET	3.1
1	D	133	THR	3.0
1	A	275	GLY	3.0
1	D	258	ILE	3.0
1	A	175	CYS	3.0
2	B	132	VAL	3.0
2	E	284	VAL	3.0
2	E	70	LEU	3.0
2	E	7	LYS	3.0
1	D	178	PRO	3.0
1	A	412	LYS	3.0
1	A	225	ALA	3.0
2	E	314	ALA	3.0
2	B	348	TYR	2.9
2	E	105	ASN	2.9
2	E	272	LEU	2.9
2	E	101	ASP	2.9
2	B	177	CYS	2.9
2	B	354	PHE	2.9
1	A	321	ALA	2.9
2	E	204	ASP	2.9
1	D	93	HIS	2.9
2	E	238	VAL	2.9
2	E	175	LEU	2.9
1	D	160	PHE	2.9
2	E	354	PHE	2.8
2	E	235	LYS	2.8
2	E	39	GLY	2.8
2	B	185	VAL	2.8
2	E	224	ALA	2.8
1	A	227	LYS	2.8
2	E	351	THR	2.8
1	D	105	TRP	2.8
2	B	192	ILE	2.8
2	E	321	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	224	VAL	2.8
1	D	146	LEU	2.7
1	D	278	LEU	2.7
2	E	252	PRO	2.7
2	E	86	SER	2.7
1	D	110	LYS	2.7
2	B	178	CYS	2.7
1	A	32	ALA	2.7
1	D	225	ALA	2.7
2	E	217	VAL	2.7
1	A	223	CYS	2.7
1	D	279	THR	2.7
1	A	270	ALA	2.7
2	E	257	PHE	2.7
1	D	48	LEU	2.7
2	B	19	LEU	2.7
2	B	352	PRO	2.7
2	B	351	THR	2.7
1	A	14	TRP	2.7
2	B	181	MET	2.7
2	B	279	PRO	2.7
2	B	282	SER	2.7
1	D	21	ILE	2.6
1	D	106	PHE	2.6
2	E	212	GLU	2.6
2	E	23	ILE	2.6
2	E	192	ILE	2.6
1	D	72	GLY	2.6
1	D	64	HIS	2.6
2	E	133	HIS	2.6
1	D	322	VAL	2.6
2	E	350	ILE	2.6
1	D	4	PRO	2.6
1	A	403	LYS	2.6
1	A	216	CYS	2.6
1	A	410	GLU	2.6
2	E	356	SER	2.6
1	D	317	PHE	2.6
1	A	391	ASN	2.6
2	E	108	GLN	2.6
1	D	223	CYS	2.6
2	E	228	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	129	PHE	2.5
1	A	408	THR	2.5
1	D	74	GLY	2.5
2	B	358	PHE	2.5
1	D	334	GLU	2.5
2	B	232	LYS	2.5
2	E	102	ASP	2.5
1	D	226	SER	2.5
1	D	257	ASP	2.5
2	E	36	VAL	2.5
2	E	172	ARG	2.5
2	E	250	MET	2.5
1	D	185	CYS	2.5
1	D	92	GLU	2.5
1	A	105	TRP	2.5
2	B	268	VAL	2.5
2	E	128	LEU	2.5
2	E	202	PRO	2.4
2	E	24	ALA	2.4
1	D	53	ILE	2.4
1	D	122	TRP	2.4
2	B	179	ALA	2.4
2	E	174	SER	2.4
1	D	90	GLU	2.4
1	D	207	MET	2.4
2	B	356	SER	2.4
1	A	235	ILE	2.4
1	D	277	GLU	2.4
2	B	131	ILE	2.4
2	B	150	ILE	2.4
1	D	102	PRO	2.4
1	D	302	GLY	2.4
2	B	61	LEU	2.4
2	E	360	ALA	2.4
2	E	135	GLN	2.4
1	D	84	LEU	2.4
1	A	258	ILE	2.4
1	D	248	ALA	2.3
1	D	249	VAL	2.3
1	A	250	LYS	2.3
1	D	137	ILE	2.3
2	E	268	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	233	ALA	2.3
1	A	315	ALA	2.3
1	D	171	THR	2.3
2	E	85	THR	2.3
2	B	269	GLY	2.3
2	E	134	THR	2.3
1	A	324	GLY	2.3
2	B	84	TRP	2.3
2	B	134	THR	2.3
2	B	173	ILE	2.3
2	E	297	PRO	2.3
2	E	215	SER	2.3
1	D	151	GLU	2.2
1	A	409	GLU	2.2
2	E	301	LYS	2.2
1	A	389	PRO	2.2
1	D	124	SER	2.2
2	E	131	ILE	2.2
1	A	325	TRP	2.2
1	D	75	GLY	2.2
2	E	116	GLY	2.2
1	D	153	LEU	2.2
1	D	55	TYR	2.2
2	B	92	PHE	2.2
1	A	388	ALA	2.2
1	D	26	GLU	2.2
2	B	176	ALA	2.2
1	D	386	VAL	2.2
2	B	183	GLY	2.2
1	D	256	MET	2.2
1	D	246	GLN	2.2
2	B	147	ALA	2.2
1	D	18	VAL	2.2
1	D	142	ARG	2.2
1	D	263	VAL	2.2
2	B	154	VAL	2.2
1	D	280	ILE	2.2
1	A	413	LYS	2.2
1	D	264	LYS	2.2
1	D	130	HIS	2.2
1	D	175	CYS	2.2
1	A	393	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	273	SER	2.1
1	D	113	ARG	2.1
2	E	103	LEU	2.1
2	E	298	THR	2.1
1	D	314	LYS	2.1
2	E	79	ASP	2.1
1	A	15	PRO	2.1
2	E	203	ASN	2.1
1	A	229	ARG	2.1
1	A	415	GLY	2.1
2	E	280	GLU	2.1
2	E	279	PRO	2.1
2	E	144	ALA	2.1
2	B	186	HIS	2.1
2	E	290	PRO	2.1
1	D	39	LYS	2.1
2	E	99	LYS	2.1
1	D	54	SER	2.1
2	B	24	ALA	2.1
1	D	365	ILE	2.1
2	B	62	LEU	2.1
2	E	307	LEU	2.1
1	A	312	GLY	2.1
1	D	362	GLY	2.1
2	E	270	GLY	2.1
2	B	58	THR	2.0
2	E	243	TYR	2.0
2	E	113	PHE	2.0
1	D	238	TRP	2.0
2	B	85	THR	2.0
2	E	38	PRO	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SRM	D	580	63/63	0.77	0.31	1.03	37,81,97,102	0
3	SRM	E	570	63/63	0.90	0.24	0.84	8,12,19,21	0
4	SF4	E	585	8/8	0.81	0.20	0.36	3,3,3,4	8
4	SF4	D	576	8/8	0.95	0.14	0.01	11,12,14,15	0
4	SF4	D	575	8/8	0.93	0.15	-0.15	12,14,15,16	0
4	SF4	E	586	8/8	0.96	0.17	-0.30	21,26,28,29	0
4	SF4	A	576	8/8	0.95	0.11	-0.49	2,4,9,9	0
3	SRM	A	580	63/63	0.94	0.12	-1.29	17,28,42,48	0
3	SRM	B	570	63/63	0.97	0.11	-1.43	4,10,20,32	0
4	SF4	B	585	8/8	0.94	0.12	-1.87	16,20,22,26	8
4	SF4	A	575	8/8	0.98	0.07	-2.84	9,16,18,18	0
4	SF4	B	586	8/8	0.97	0.05	-3.92	15,18,21,22	0
5	CMO	A	590	2/2	0.81	0.49	-	29,29,29,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.