



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3MM7
Title : Dissimilatory sulfite reductase carbon monoxide complex
Authors : Parey, K.; Warkentin, E.; Kroneck, P.M.H.; Ermler, U.
Deposited on : 2010-04-19
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

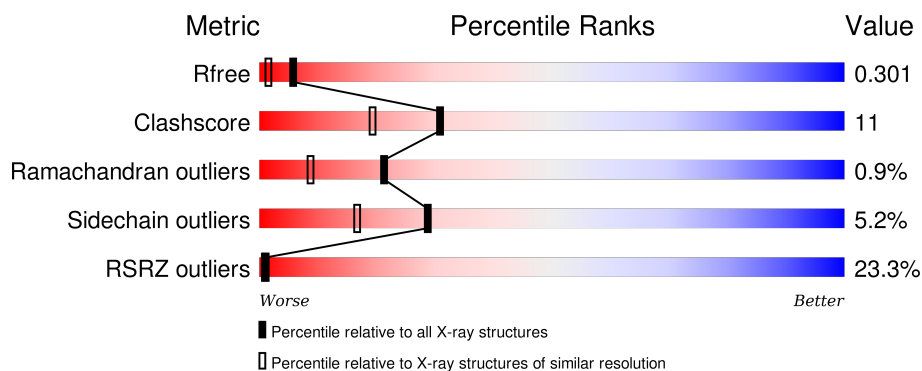
1 Overall quality at a glance ⓘ

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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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>13%</div> <div>79%</div> <div>16%</div> <div>• •</div> </div>
1	D	418	<div> <div>29%</div> <div>84%</div> <div>15%</div> <div></div> </div>
2	B	366	<div> <div>13%</div> <div>82%</div> <div>16%</div> <div>• • •</div> </div>
2	E	366	<div> <div>39%</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.

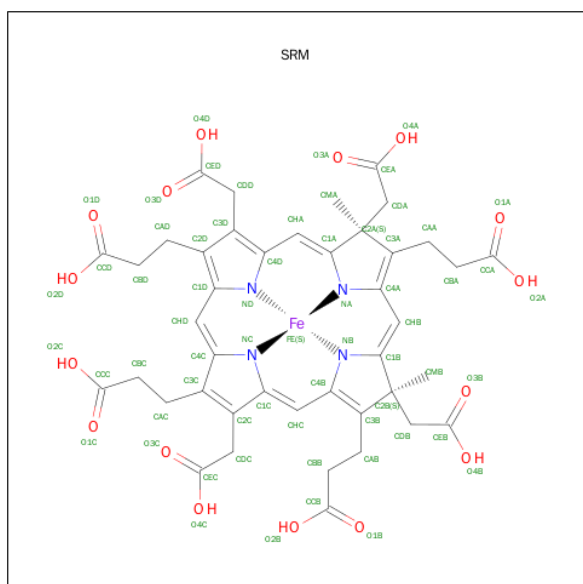
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

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.

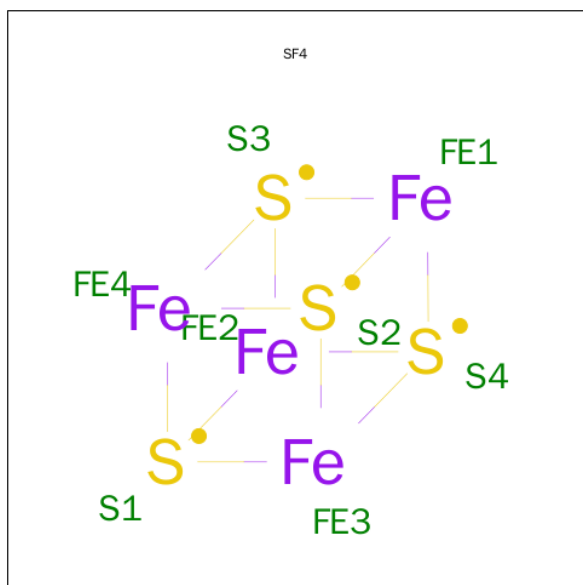
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			
2	E	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			

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



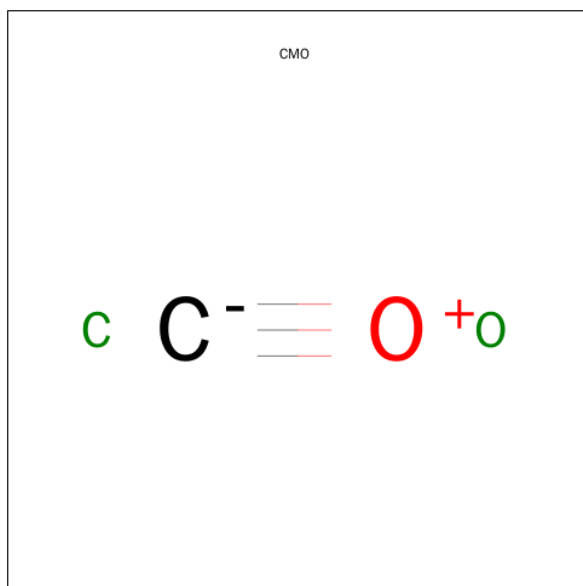
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	B	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	D	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	E	1	Total	C	Fe	N	O	
			63	42	1	4	16	

- 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		

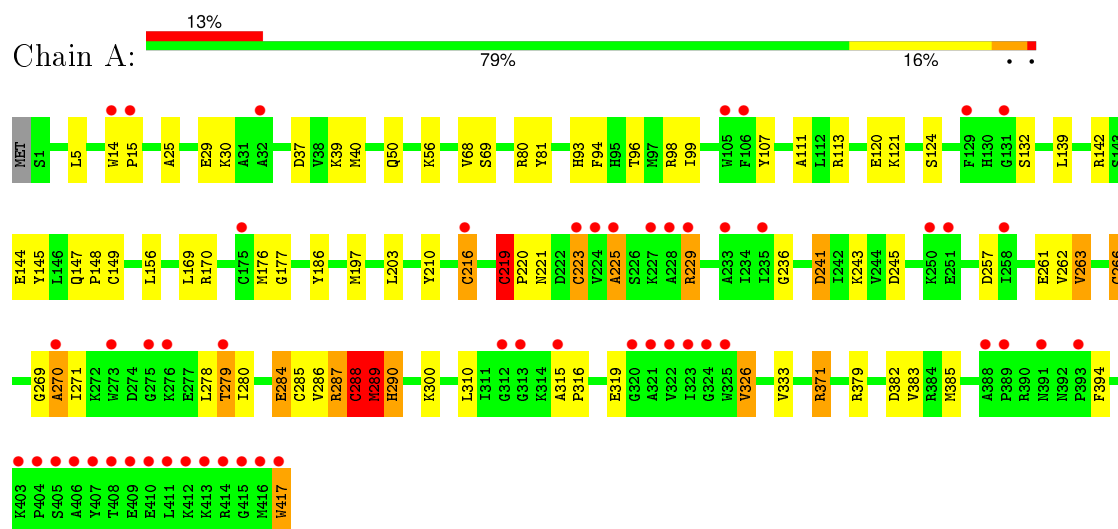
- Molecule 6 is water.

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		

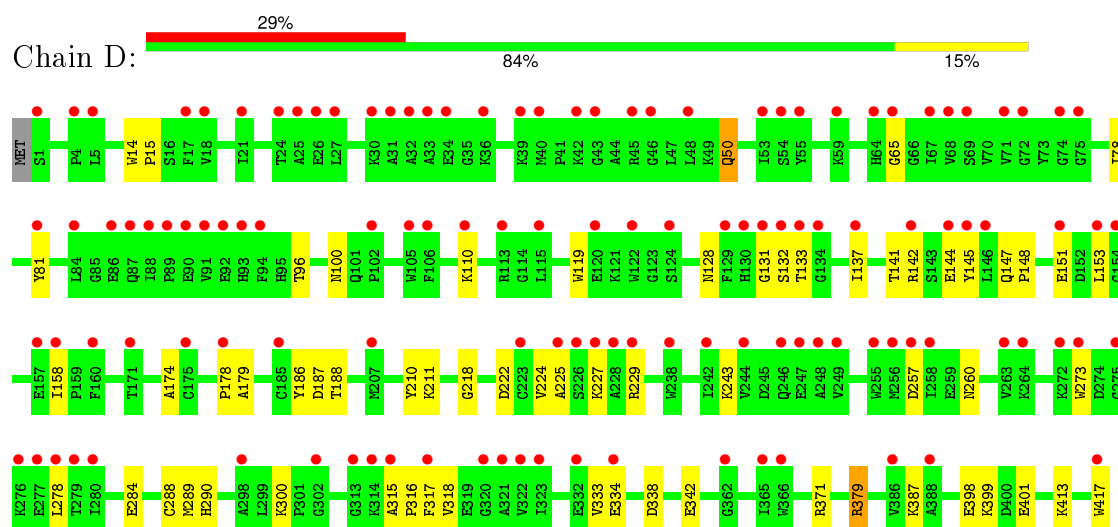
3 Residue-property plots [i](#)

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

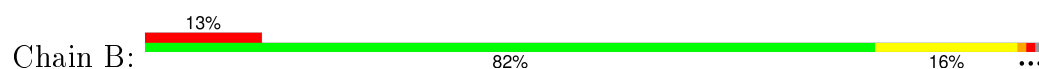
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

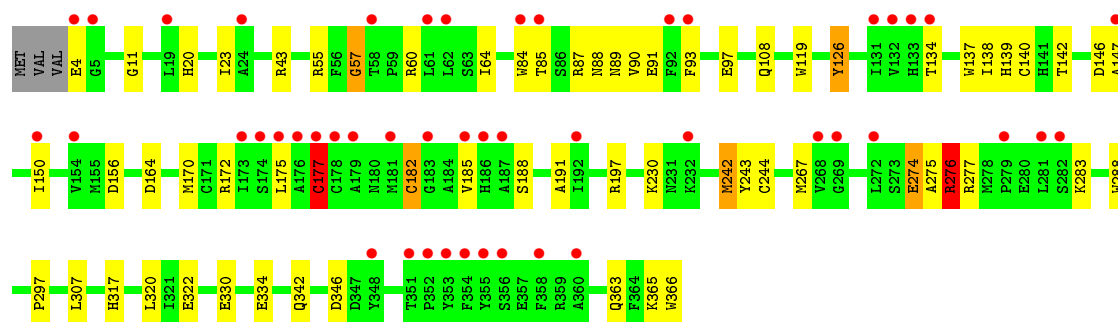


- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

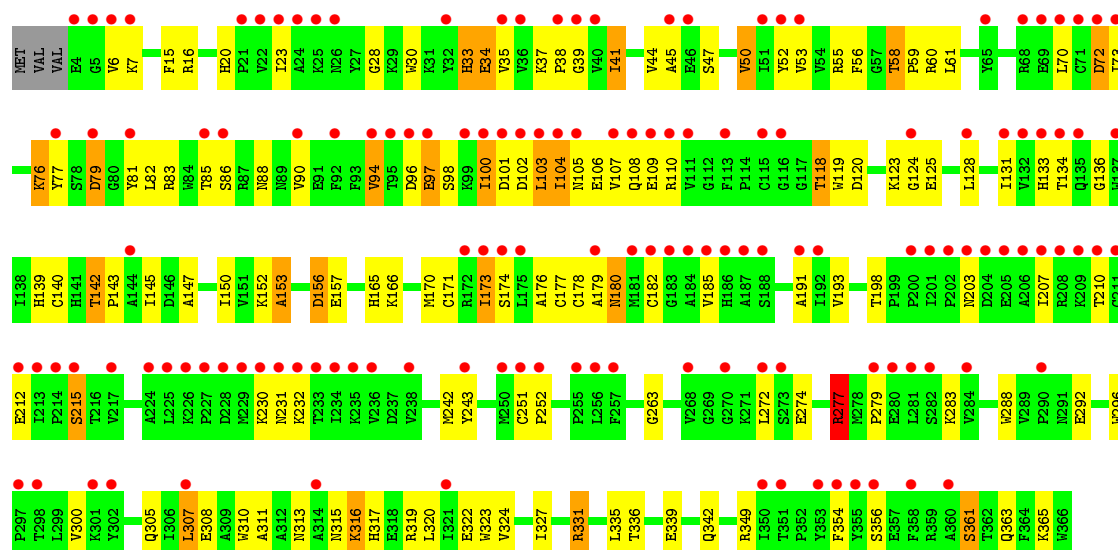
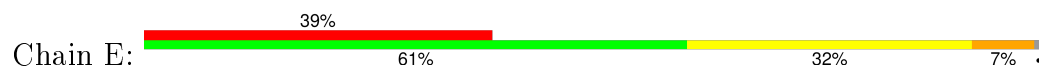


- Molecule 2: Sulfite reductase, dissimilatory-type subunit beta





- 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
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 140628 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:94:VAL:HG12	2:E:96:ASP:H	1.55	0.70
2:E:263:GLY:HA3	2:E:288:TRP:NE1	2.07	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
2:E:37:LYS:HB2	2:E:38:PRO:HD2	1.82	0.61
1:D:243:LYS:HE3	1:D:300:LYS:HE3	1.81	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:E:272:LEU:HB2	3:E:570:SRM:CCC	2.34	0.57
2:B:276:ARG:HG3	2:B:276:ARG:NH1	2.18	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
2:E:323:TRP:NE1	2:E:327:ILE:HD13	2.21	0.56
1:D:151:GLU:HG2	2:E:6:VAL:HG22	1.87	0.56
3:D:580:SRM:HMB1	3:D:580:SRM:CBB	2.32	0.56
2:E:97:GLU:O	2:E:100:ILE:HD11	2.06	0.56
2:E:145:ILE:HB	2:E:150:ILE:HD11	1.87	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)
1:D:128:ASN:HD22	2:E:61:LEU:HA	1.72	0.55
2:E:157:GLU:HG3	2:E:300:VAL:HG11	1.87	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
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
1:A:98:ARG:C	1:A:99:ILE:HD13	2.28	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: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
1:A:223:CYS:HB3	3:B:570:SRM:CHC	2.39	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
2:E:320:LEU:O	2:E:324:VAL:HG23	2.10	0.51
1:D:186:TYR:CD1	1:D:333:VAL:HG11	2.46	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
2:E:110:ARG:N	6:E:498:HOH:O	2.28	0.50
1:A:300:LYS:HD3	6:B:571:HOH:O	2.10	0.50
1:D:338:ASP:O	1:D:342:GLU:HB2	2.12	0.50
2:E:263:GLY:HA3	2:E:288:TRP:HE1	1.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ASP:O	1:A:261:GLU:HB2	2.12	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:230:LYS:CA	2:E:231:ASN:HB2	2.42	0.49
2:E:103:LEU:O	2:E:106:GLU:N	2.45	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:85:THR:HB	3:E:570:SRM:HAB2	1.98	0.46
2:E:131:ILE:HG23	2:E:174:SER:HA	1.97	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:72:ASP:CG	2:E:72:ASP:CA	2.76	0.45
2:E:15:PHE:CG	2:E:16:ARG:N	2.84	0.45
2:B:138:ILE:HG13	6:B:379:HOH:O	2.15	0.45
3:E:570:SRM:HHA	3:E:570:SRM:HMA2	1.72	0.45
1:A:81:TYR:HE2	1:A:93:HIS:CE1	2.34	0.45
2:E:55:ARG:NH2	3:E:570:SRM:HBA2	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:GLN:HE21	1:D:50:GLN:HB2	1.60	0.45
1:A:241:ASP:N	1:A:241:ASP:OD1	2.47	0.45
1:D:225:ALA:HB3	1:D:229:ARG:HD3	1.97	0.45
2:E:134:THR:CG2	2:E:182:CYS:CB	2.77	0.45
1:A:326:VAL:HB	1:A:385:MET:HA	1.98	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
2:E:103:LEU:O	2:E:104:ILE:C	2.56	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
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:E:73:ILE:HD11	2:E:110:ARG:HD3	2.00	0.43
2:B:322:GLU:OE1	6:B:420:HOH:O	2.21	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:387:LYS:HB2	1:D:387:LYS:HE2	1.79	0.43
1:D:153:LEU:HD23	1:D:153:LEU:HA	1.88	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
2:E:58:THR:C	2:E:60:ARG:H	2.22	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
1:D:110:LYS:HD2	1:D:158:ILE:HD12	2.00	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:E:37:LYS:HB2	2:E:38:PRO:CD	2.49	0.42
2:B:175:LEU:C	2:B:175:LEU:HD23	2.39	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
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
2:B:146:ASP:O	2:B:150:ILE:HD12	2.19	0.42
1:A:37:ASP:OD2	1:A:121:LYS:HE3	2.19	0.42
1:A:176:MET:HG2	4:A:575:SF4:S1	2.60	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:E:58:THR:HG23	2:E:88:ASN:O	2.20	0.41
1:D:290:HIS:N	6:D:540:HOH:O	2.36	0.41
2:B:90:VAL:HG22	2:B:91:GLU:N	2.35	0.41
2:E:128:LEU:HD12	2:E:171:CYS:O	2.19	0.41
3:E:570:SRM:HMA3	3:E:570:SRM:HAA2	1.56	0.41
2:E:307:LEU:HD23	2:E:308:GLU:HG3	2.02	0.41
2:E:203:ASN:O	2:E:207:ILE:HG13	2.19	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:D:128:ASN:HD21	2:E:61:LEU:CD1	2.33	0.41
1:A:417:TRP:HD1	1:A:417:TRP:C	2.22	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:HD23	2:E:320:LEU:C	2.41	0.41
2:B:57:GLY:HA2	2:B:89:ASN:OD1	2.21	0.40
1:A:271:ILE:HA	1:A:279:THR:O	2.21	0.40
1:A:186:TYR:CD1	1:A:333:VAL:HG11	2.56	0.40
2:E:177:CYS:CB	4:E:585:SF4:S3	2.99	0.40
2:E:316:LYS:HG3	2:E:317:HIS:CD2	2.56	0.40
2:E:35:VAL:HG21	2:E:119:TRP:O	2.22	0.40
2:B:191:ALA:HB3	2:B:267:MET:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:342:GLN:OE1	2:E:342:GLN:C	2.60	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%)	34	21
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%)	21	9

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%)	34	21
1	D	353/354 (100%)	343 (97%)	10 (3%)	51	41
2	B	314/317 (99%)	301 (96%)	13 (4%)	37	25
2	E	314/317 (99%)	284 (90%)	30 (10%)	10	3
All	All	1334/1342 (99%)	1265 (95%)	69 (5%)	29	17

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	29,70,70	2.13	7 (24%)	29,112,112	3.89	13 (44%)
5	CMO	A	590	-	0,1,1	0.00	-	0,0,0	0.00	-
3	SRM	B	570	1	29,70,70	2.96	12 (41%)	29,112,112	8.59	21 (72%)
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	-	29,70,70	2.08	7 (24%)	29,112,112	3.88	13 (44%)
3	SRM	E	570	1	29,70,70	2.60	10 (34%)	29,112,112	4.66	17 (58%)
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 (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	570	SRM	C4B-NB	-7.37	1.25	1.39
3	B	570	SRM	C1B-NB	-6.76	1.28	1.38
3	B	570	SRM	C4C-NC	-6.54	1.27	1.36
3	E	570	SRM	C1C-NC	-4.78	1.30	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	570	SRM	C4C-NC	-4.55	1.30	1.36
3	E	570	SRM	C4A-NA	-4.38	1.30	1.39
3	B	570	SRM	C4A-NA	-3.79	1.31	1.39
3	E	570	SRM	C1B-NB	-3.50	1.32	1.38
3	D	580	SRM	C4A-NA	-3.03	1.33	1.39
3	A	580	SRM	C4A-NA	-2.76	1.33	1.39
3	B	570	SRM	C1D-CHD	-2.66	1.32	1.39
3	D	580	SRM	C1A-NA	-2.53	1.34	1.38
3	E	570	SRM	C1A-NA	-2.45	1.34	1.38
3	B	570	SRM	CHC-C4B	-2.39	1.33	1.39
3	E	570	SRM	CDA-C2A	-2.33	1.52	1.56
3	A	580	SRM	CAB-C3B	2.02	1.55	1.51
3	B	570	SRM	CDD-C3D	2.04	1.57	1.52
3	E	570	SRM	CDC-C2C	2.16	1.55	1.52
3	D	580	SRM	CAD-C2D	2.24	1.55	1.52
3	B	570	SRM	CDA-C2A	2.36	1.60	1.56
3	A	580	SRM	CAD-C2D	2.50	1.56	1.52
3	B	570	SRM	C3C-C2C	3.10	1.46	1.37
3	E	570	SRM	CAD-C2D	3.14	1.57	1.52
3	B	570	SRM	C1A-NA	3.23	1.43	1.38
3	D	580	SRM	FE-NA	3.54	2.09	1.95
3	D	580	SRM	FE-NB	3.76	2.10	1.95
3	B	570	SRM	C3D-C2D	4.12	1.48	1.39
3	D	580	SRM	C3C-C2C	4.19	1.50	1.37
3	A	580	SRM	FE-NB	4.20	2.12	1.95
3	B	570	SRM	CHB-C4A	4.51	1.49	1.39
3	A	580	SRM	FE-NA	4.51	2.13	1.95
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	6.55	1.54	1.39
3	D	580	SRM	C3D-C2D	6.73	1.54	1.39
3	E	570	SRM	C3D-C2D	7.09	1.55	1.39

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	SRM	C4A-NA-C1A	-20.36	95.85	106.90
3	B	570	SRM	CAA-C3A-C2A	-19.90	101.06	123.46
3	B	570	SRM	CAB-C3B-C2B	-17.19	104.10	123.46
3	A	580	SRM	CAB-C3B-C2B	-15.02	106.55	123.46
3	E	570	SRM	CAA-C3A-C2A	-13.00	108.83	123.46
3	D	580	SRM	CDD-C3D-C4D	-10.81	109.78	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	SRM	C3B-C4B-NB	-10.17	98.78	110.09
3	E	570	SRM	CAD-C2D-C1D	-9.86	116.30	127.01
3	E	570	SRM	C4A-NA-C1A	-8.19	102.45	106.90
3	E	570	SRM	CAC-C3C-C4C	-7.26	119.13	127.01
3	D	580	SRM	CAB-C3B-C2B	-6.82	115.79	123.46
3	B	570	SRM	CEC-CDC-C2C	-6.32	104.24	116.31
3	D	580	SRM	CAD-C2D-C1D	-5.83	120.68	127.01
3	D	580	SRM	CAD-C2D-C3D	-5.49	115.71	129.38
3	B	570	SRM	CAD-C2D-C1D	-5.12	121.45	127.01
3	D	580	SRM	CAA-C3A-C2A	-4.45	118.45	123.46
3	E	570	SRM	CEC-CDC-C2C	-4.41	107.88	116.31
3	E	570	SRM	CBC-CAC-C3C	-4.39	104.66	112.53
3	E	570	SRM	CDC-C2C-C1C	-4.29	120.46	127.38
3	B	570	SRM	CAC-CBC-CCC	-4.19	105.07	112.75
3	B	570	SRM	CBC-CAC-C3C	-4.19	105.02	112.53
3	A	580	SRM	CAA-C3A-C2A	-4.09	118.86	123.46
3	E	570	SRM	CAC-C3C-C2C	-3.72	120.11	129.38
3	E	570	SRM	CHB-C4A-C3A	-3.64	117.21	125.48
3	B	570	SRM	CHB-C4A-C3A	-3.58	117.35	125.48
3	D	580	SRM	C4B-NB-C1B	-3.35	105.08	106.90
3	D	580	SRM	C3A-C4A-NA	-3.11	106.63	110.09
3	E	570	SRM	CAB-C3B-C2B	-2.95	120.15	123.46
3	D	580	SRM	CAA-CBA-CCA	-2.64	107.91	112.75
3	A	580	SRM	CAC-CBC-CCC	-2.52	108.13	112.75
3	A	580	SRM	CMB-C2B-CDB	-2.49	106.80	109.76
3	A	580	SRM	C4B-NB-C1B	-2.46	105.57	106.90
3	A	580	SRM	CAD-C2D-C3D	-2.36	123.52	129.38
3	E	570	SRM	CDD-C3D-C4D	-2.14	123.86	127.34
3	E	570	SRM	CAB-CBB-CCB	2.01	116.42	112.75
3	D	580	SRM	CDC-C2C-C1C	2.03	130.66	127.38
3	B	570	SRM	CAB-CBB-CCB	2.24	116.84	112.75
3	E	570	SRM	CAA-CBA-CCA	2.38	117.12	112.75
3	B	570	SRM	CMB-C2B-CDB	2.40	112.62	109.76
3	A	580	SRM	CDC-C2C-C1C	2.43	131.30	127.38
3	A	580	SRM	C3B-C4B-NB	2.63	113.01	110.09
3	D	580	SRM	C3B-C4B-NB	2.81	113.21	110.09
3	B	570	SRM	CAC-C3C-C4C	3.06	130.33	127.01
3	B	570	SRM	C2A-CDA-CEA	3.21	120.42	115.45
3	E	570	SRM	CED-CDD-C3D	3.35	122.71	116.31
3	E	570	SRM	C2B-CDB-CEB	3.35	120.65	115.45
3	B	570	SRM	CDD-C3D-C4D	3.48	133.00	127.34
3	B	570	SRM	CDC-C2C-C1C	4.14	134.07	127.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	SRM	C1C-CHC-C4B	4.31	138.47	124.39
3	D	580	SRM	CBD-CAD-C2D	4.39	120.39	112.53
3	A	580	SRM	CMA-C2A-CDA	4.46	115.07	109.76
3	A	580	SRM	C4A-NA-C1A	4.54	109.37	106.90
3	B	570	SRM	CHC-C4B-NB	5.02	133.49	123.70
3	A	580	SRM	CAC-C3C-C4C	5.40	132.87	127.01
3	A	580	SRM	C2A-CDA-CEA	5.72	124.32	115.45
3	E	570	SRM	CBD-CAD-C2D	6.47	124.12	112.53
3	A	580	SRM	CBD-CAD-C2D	6.73	124.60	112.53
3	E	570	SRM	C3A-C4A-NA	7.18	118.08	110.09
3	B	570	SRM	CMA-C2A-CDA	7.24	118.38	109.76
3	D	580	SRM	CMA-C2A-CDA	7.53	118.72	109.76
3	D	580	SRM	C4A-NA-C1A	7.85	111.16	106.90
3	B	570	SRM	CBD-CAD-C2D	9.77	130.05	112.53
3	B	570	SRM	C3A-C4A-NA	10.75	122.03	110.09
3	B	570	SRM	C4B-NB-C1B	20.76	118.17	106.90

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.77	53 (12%) 5 5	4, 17, 30, 66	0
1	D	417/418 (99%)	1.58	123 (29%) 1 0	7, 15, 28, 38	0
2	B	363/366 (99%)	0.83	47 (12%) 5 5	8, 17, 26, 51	0
2	E	363/366 (99%)	1.87	141 (38%) 0 0	2, 12, 36, 55	0
All	All	1560/1568 (99%)	1.25	364 (23%) 1 1	2, 16, 30, 66	0

All (364) 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	8.6
1	D	67	ILE	8.3
2	E	184	ALA	8.1
1	D	91	VAL	7.6
1	D	33	ALA	7.6
1	D	25	ALA	7.3
2	E	234	ILE	6.9
2	E	183	GLY	6.9
1	D	32	ALA	6.8
1	D	88	ILE	6.8
2	E	5	GLY	6.7
2	E	206	ALA	6.5
2	E	100	ILE	6.5
1	D	31	ALA	5.9
1	D	30	LYS	5.9
1	D	1	SER	5.8
2	E	207	ILE	5.6
1	D	276	LYS	5.6
2	E	233	THR	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	406	ALA	5.5
1	D	5	LEU	5.5
2	E	6	VAL	5.4
2	E	40	VAL	5.4
1	A	416	MET	5.4
1	D	94	PHE	5.4
2	E	77	TYR	5.3
2	E	232	LYS	5.2
1	A	417	TRP	5.2
2	E	185	VAL	5.1
2	E	35	VAL	5.0
2	E	51	ILE	5.0
2	E	111	VAL	5.0
2	E	201	ILE	4.9
2	E	109	GLU	4.9
2	B	5	GLY	4.9
2	E	209	LYS	4.9
1	D	228	ALA	4.8
2	E	187	ALA	4.8
2	E	95	THR	4.6
2	B	272	LEU	4.6
2	E	225	LEU	4.6
1	D	158	ILE	4.6
2	E	236	VAL	4.5
1	D	132	SER	4.5
1	D	157	GLU	4.5
2	E	205	GLU	4.5
1	D	255	TRP	4.4
2	E	355	TYR	4.4
2	B	4	GLU	4.3
1	D	315	ALA	4.3
1	D	86	GLU	4.2
2	E	281	LEU	4.2
1	D	40	MET	4.2
2	E	211	CYS	4.1
2	E	25	LYS	4.1
1	D	229	ARG	4.1
2	E	182	CYS	4.1
1	D	42	LYS	4.1
2	B	355	TYR	4.1
2	E	132	VAL	4.0
1	A	313	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	353	TYR	4.0
1	D	273	TRP	4.0
2	E	256	LEU	4.0
1	A	273	TRP	4.0
1	A	407	TYR	4.0
2	E	69	GLU	4.0
2	B	175	LEU	4.0
2	E	213	ILE	4.0
1	D	65	GLY	4.0
2	E	115	CYS	3.9
1	D	131	GLY	3.9
2	E	124	GLY	3.9
2	E	210	THR	3.9
1	D	45	ARG	3.9
2	E	53	VAL	3.9
2	E	97	GLU	3.9
1	D	43	GLY	3.9
2	E	251	CYS	3.9
1	A	404	PRO	3.9
1	D	24	THR	3.9
2	E	302	TYR	3.8
2	E	71	CYS	3.8
1	A	228	ALA	3.8
1	D	145	TYR	3.8
2	E	188	SER	3.7
1	D	27	LEU	3.7
1	D	323	ILE	3.7
2	E	90	VAL	3.7
1	A	279	THR	3.7
2	E	96	ASP	3.7
1	A	106	PHE	3.7
2	E	230	LYS	3.7
1	D	332	GLU	3.7
2	E	21	PRO	3.7
2	E	104	ILE	3.6
1	D	59	LYS	3.6
2	E	110	ARG	3.6
2	E	107	VAL	3.6
2	E	32	TYR	3.6
1	A	276	LYS	3.6
1	D	321	ALA	3.5
2	E	214	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	68	VAL	3.5
2	E	200	PRO	3.5
2	E	94	VAL	3.5
2	E	226	LYS	3.5
2	E	208	ARG	3.5
1	D	71	VAL	3.5
1	D	89	PRO	3.4
2	E	353	TYR	3.4
2	E	92	PHE	3.4
1	D	134	GLY	3.4
1	D	144	GLU	3.4
1	A	411	LEU	3.4
1	D	69	SER	3.4
2	E	45	ALA	3.4
2	E	73	ILE	3.4
1	D	417	TRP	3.4
1	D	247	GLU	3.4
1	D	313	GLY	3.4
2	B	281	LEU	3.4
2	E	255	PRO	3.4
1	D	320	GLY	3.4
2	E	72	ASP	3.4
2	E	65	TYR	3.4
2	E	227	PRO	3.3
1	D	272	LYS	3.3
1	D	154	GLY	3.3
1	D	227	LYS	3.3
1	D	87	GLN	3.3
1	D	244	VAL	3.3
1	D	275	GLY	3.3
1	A	322	VAL	3.3
2	E	186	HIS	3.3
2	E	81	TYR	3.3
1	A	405	SER	3.3
2	E	26	ASN	3.3
2	E	68	ARG	3.2
2	B	187	ALA	3.2
2	E	52	TYR	3.2
2	E	137	TRP	3.2
1	D	115	LEU	3.2
2	E	358	PHE	3.2
1	A	323	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	36	LYS	3.2
2	E	282	SER	3.2
1	A	414	ARG	3.1
1	D	366	TRP	3.1
2	B	174	SER	3.1
2	E	231	ASN	3.1
1	D	258	ILE	3.1
2	E	46	GLU	3.1
1	A	275	GLY	3.1
1	D	133	THR	3.1
2	B	132	VAL	3.1
2	E	284	VAL	3.1
2	E	70	LEU	3.1
2	E	181	MET	3.1
1	A	175	CYS	3.1
1	A	225	ALA	3.0
2	E	314	ALA	3.0
1	D	178	PRO	3.0
2	E	7	LYS	3.0
1	A	412	LYS	3.0
2	E	272	LEU	3.0
2	B	348	TYR	3.0
2	B	354	PHE	3.0
2	E	105	ASN	3.0
2	E	238	VAL	3.0
1	A	321	ALA	3.0
2	B	177	CYS	3.0
2	E	101	ASP	3.0
2	E	175	LEU	3.0
1	D	160	PHE	2.9
2	E	204	ASP	2.9
1	D	93	HIS	2.9
2	B	185	VAL	2.9
2	E	354	PHE	2.9
2	E	224	ALA	2.9
2	E	39	GLY	2.9
2	B	192	ILE	2.9
2	E	321	ILE	2.9
2	E	351	THR	2.9
1	A	224	VAL	2.9
1	D	105	TRP	2.9
2	E	235	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	227	LYS	2.8
1	D	146	LEU	2.8
1	D	278	LEU	2.8
2	E	217	VAL	2.8
1	A	32	ALA	2.8
1	D	225	ALA	2.8
2	E	252	PRO	2.8
2	E	86	SER	2.8
2	B	178	CYS	2.8
2	E	257	PHE	2.8
1	A	223	CYS	2.8
1	A	270	ALA	2.8
1	D	48	LEU	2.8
2	B	19	LEU	2.8
1	D	110	LYS	2.8
1	D	279	THR	2.7
1	D	21	ILE	2.7
2	B	352	PRO	2.7
1	D	106	PHE	2.7
2	B	351	THR	2.7
1	A	14	TRP	2.7
2	E	23	ILE	2.7
2	E	192	ILE	2.7
1	D	322	VAL	2.7
2	B	279	PRO	2.7
2	B	282	SER	2.7
2	E	350	ILE	2.7
1	D	72	GLY	2.7
2	B	181	MET	2.7
1	D	64	HIS	2.7
2	E	133	HIS	2.7
2	E	212	GLU	2.7
1	D	317	PHE	2.7
1	D	4	PRO	2.7
1	A	216	CYS	2.6
2	E	356	SER	2.6
1	D	129	PHE	2.6
1	D	223	CYS	2.6
1	A	403	LYS	2.6
1	A	391	ASN	2.6
1	A	410	GLU	2.6
2	E	228	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	358	PHE	2.6
2	E	108	GLN	2.6
1	D	74	GLY	2.6
1	A	408	THR	2.6
2	E	36	VAL	2.6
2	E	102	ASP	2.6
1	D	334	GLU	2.6
2	B	268	VAL	2.6
1	D	226	SER	2.6
1	D	257	ASP	2.6
1	D	185	CYS	2.5
2	B	232	LYS	2.5
2	E	128	LEU	2.5
1	D	53	ILE	2.5
1	A	105	TRP	2.5
2	E	24	ALA	2.5
2	E	172	ARG	2.5
2	E	250	MET	2.5
2	E	202	PRO	2.5
1	D	92	GLU	2.5
2	B	179	ALA	2.5
1	D	122	TRP	2.5
1	A	235	ILE	2.5
2	B	131	ILE	2.5
2	B	150	ILE	2.5
2	E	174	SER	2.5
2	B	61	LEU	2.5
2	B	356	SER	2.5
2	E	360	ALA	2.5
1	D	302	GLY	2.5
1	D	84	LEU	2.5
1	D	102	PRO	2.5
1	D	90	GLU	2.4
1	A	258	ILE	2.4
1	D	277	GLU	2.4
1	D	207	MET	2.4
1	D	249	VAL	2.4
1	D	248	ALA	2.4
2	E	135	GLN	2.4
2	E	268	VAL	2.4
1	D	137	ILE	2.4
1	A	233	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	315	ALA	2.4
1	A	250	LYS	2.4
1	D	171	THR	2.4
2	E	85	THR	2.4
2	B	173	ILE	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	E	297	PRO	2.3
2	E	215	SER	2.3
2	B	134	THR	2.3
2	E	131	ILE	2.3
1	D	153	LEU	2.3
1	D	386	VAL	2.3
2	B	92	PHE	2.3
1	A	389	PRO	2.3
1	D	124	SER	2.3
1	D	151	GLU	2.3
1	A	388	ALA	2.3
1	D	75	GLY	2.3
2	B	176	ALA	2.3
2	E	116	GLY	2.3
1	A	325	TRP	2.3
1	D	18	VAL	2.3
1	D	263	VAL	2.3
2	B	154	VAL	2.3
1	A	409	GLU	2.3
1	D	280	ILE	2.3
2	B	183	GLY	2.3
2	E	301	LYS	2.3
2	B	147	ALA	2.3
1	D	55	TYR	2.3
1	D	26	GLU	2.2
2	E	103	LEU	2.2
1	D	246	GLN	2.2
1	D	175	CYS	2.2
1	D	130	HIS	2.2
1	D	256	MET	2.2
2	E	273	SER	2.2
1	A	393	PRO	2.2
1	D	142	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	413	LYS	2.2
1	D	264	LYS	2.2
2	E	79	ASP	2.2
2	E	298	THR	2.2
1	A	15	PRO	2.2
1	D	113	ARG	2.2
1	D	314	LYS	2.2
1	A	415	GLY	2.2
2	E	203	ASN	2.2
2	E	144	ALA	2.1
2	E	279	PRO	2.1
1	A	229	ARG	2.1
1	D	365	ILE	2.1
2	B	62	LEU	2.1
2	E	280	GLU	2.1
2	E	307	LEU	2.1
2	B	24	ALA	2.1
2	E	290	PRO	2.1
2	B	186	HIS	2.1
2	E	113	PHE	2.1
1	D	54	SER	2.1
1	A	312	GLY	2.1
1	D	362	GLY	2.1
2	E	270	GLY	2.1
2	B	58	THR	2.1
1	D	39	LYS	2.1
1	D	238	TRP	2.1
2	E	99	LYS	2.1
2	E	243	TYR	2.1
2	E	22	VAL	2.1
2	B	85	THR	2.1
2	E	38	PRO	2.1
1	D	388	ALA	2.1
1	D	242	ILE	2.0
2	B	93	PHE	2.0
2	B	360	ALA	2.0
2	E	173	ILE	2.0
2	B	133	HIS	2.0
1	D	298	ALA	2.0
2	E	179	ALA	2.0
2	E	191	ALA	2.0
1	A	129	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	17	PHE	2.0
1	A	320	GLY	2.0
1	D	34	GLU	2.0
1	D	46	GLY	2.0
1	D	120	GLU	2.0
1	A	251	GLU	2.0
1	A	131	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.