



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:24 AM GMT

PDB ID : 3OR2  
Title : Crystal structure of dissimilatory sulfite reductase II (DsrII)  
Authors : Hsieh, Y.C.; Liu, M.Y.; Wang, V.C.C.; Chiang, Y.L.; Liu, E.H.; Wu, W.G.;  
Chan, S.I.; Chen, C.J.  
Deposited on : 2010-09-06  
Resolution : 2.05 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](mailto: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.

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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

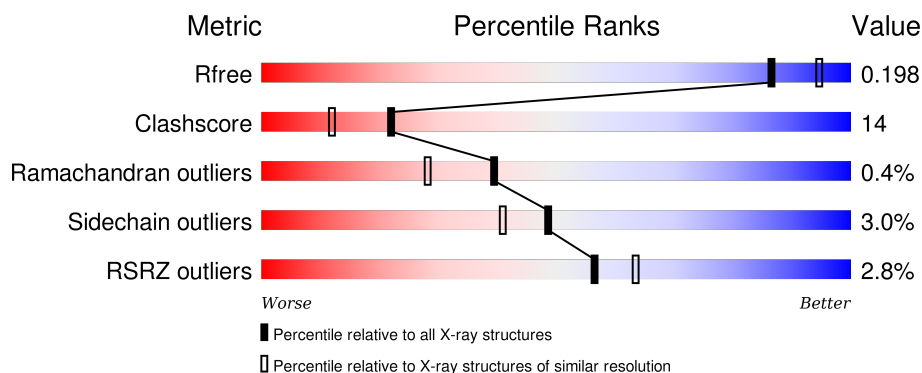
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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  $\geq 3$ , 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	435	<div> <div>71%</div> <div>27%</div> <div>•</div> </div>
1	D	435	<div> <div>72%</div> <div>25%</div> <div>•</div> </div>
2	B	385	<div> <div>2%</div> <div>78%</div> <div>19%</div> <div>••</div> </div>
2	E	385	<div> <div>76%</div> <div>23%</div> <div>•</div> </div>
3	C	104	<div> <div>22%</div> <div>68%</div> <div>27%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	104	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	B	803	-	-	X	-
5	SO3	A	6573	-	-	X	X
5	SO3	D	6575	-	-	-	X
6	SRM	B	581	-	-	-	X
6	SRM	E	583	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15433 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3421	2163	585	645	28			
1	D	435	Total	C	N	O	S	0	0	0
			3421	2163	585	645	28			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	385	Total	C	N	O	S	3	1	0
			3001	1914	519	541	27			
2	E	385	Total	C	N	O	S	0	0	0
			2998	1912	519	541	26			

- Molecule 3 is a protein called Sulfite reductase subunit gama.

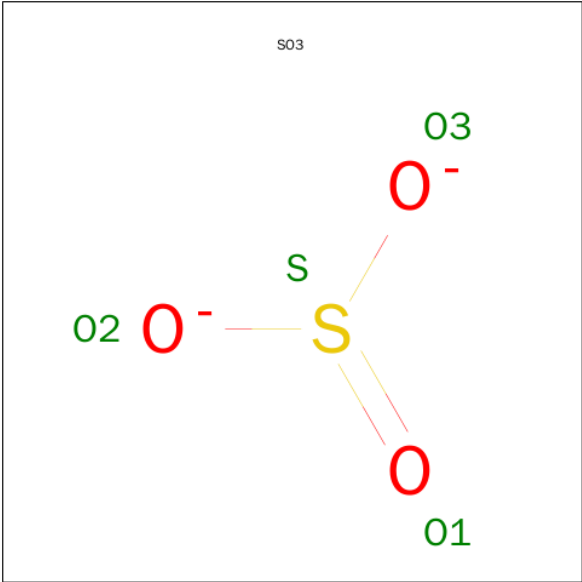
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	104	Total	C	N	O	S	3	1	0
			793	514	126	147	6			
3	F	104	Total	C	N	O	S	0	0	0
			790	512	126	147	5			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



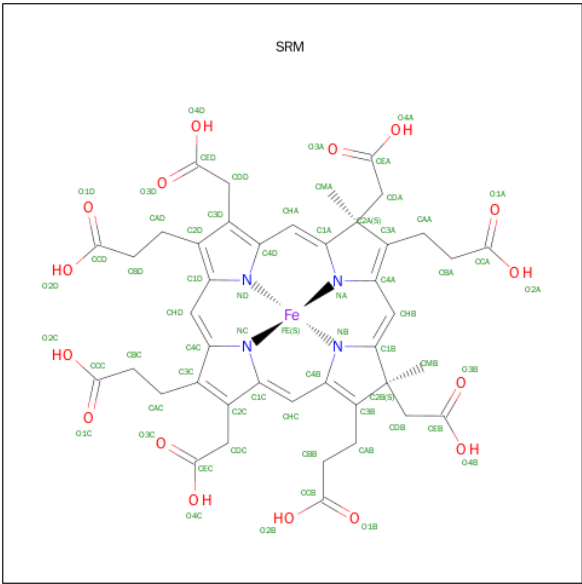
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			7	3	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			7	3	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is SULFITE ION (three-letter code: SO<sub>3</sub>) (formula: O<sub>3</sub>S).



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

- Molecule 6 is SIROHEME (three-letter code: SRM) (formula: C<sub>42</sub>H<sub>42</sub>FeN<sub>4</sub>O<sub>16</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C Fe N O 63 42 1 4 16	0	0
6	B	1	Total C N O 62 42 4 16	0	0
6	D	1	Total C Fe N O 63 42 1 4 16	0	0
6	E	1	Total C N O 62 42 4 16	0	0

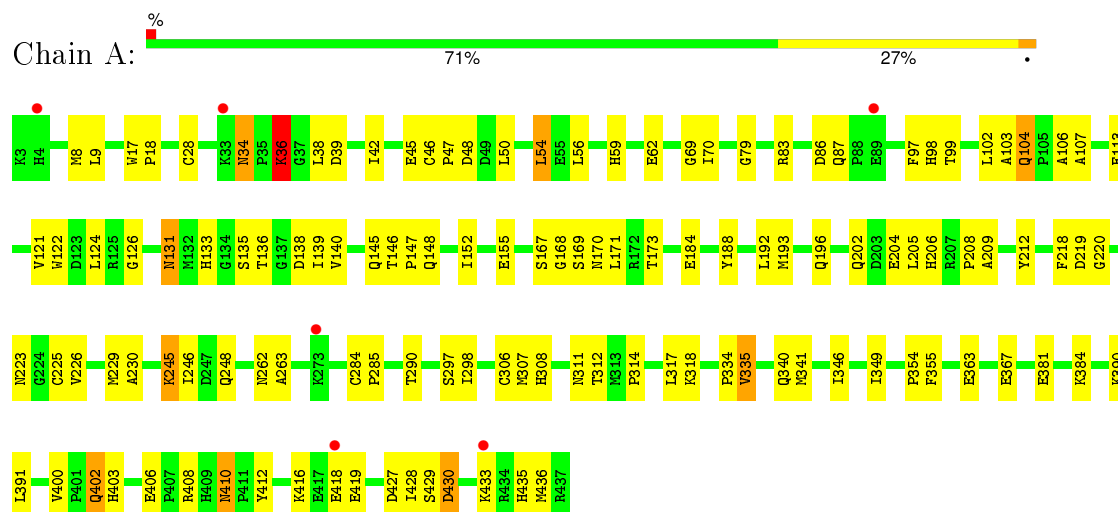
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	157	Total O 157 157	0	0
7	B	139	Total O 139 139	0	0
7	C	8	Total O 8 8	0	0
7	D	212	Total O 212 212	0	0
7	E	149	Total O 149 149	0	0
7	F	16	Total O 16 16	0	0

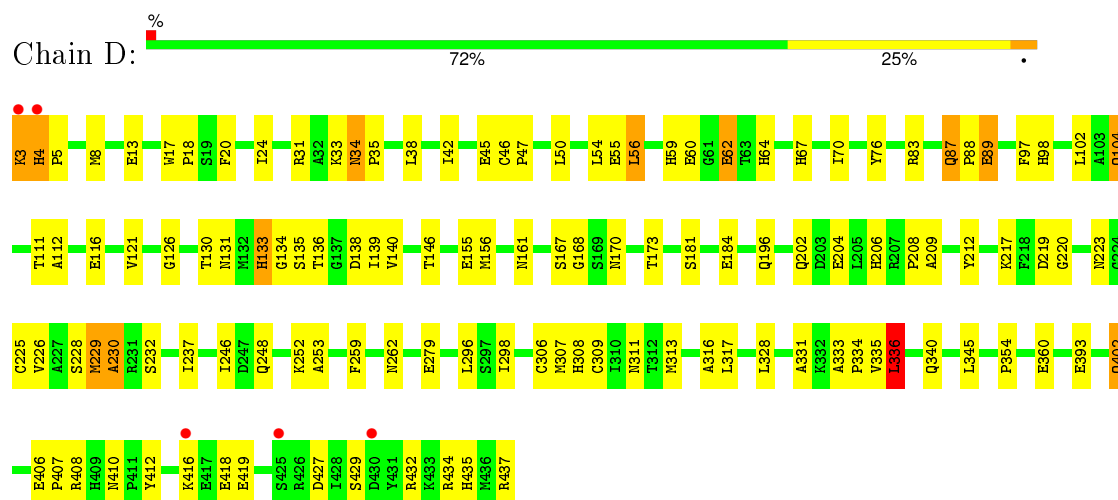
### 3 Residue-property plots

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.

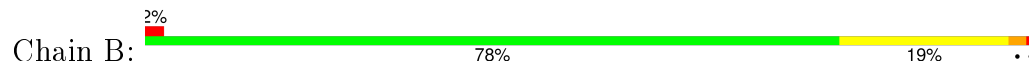
#### • Molecule 1: Sulfite reductase subunit alpha



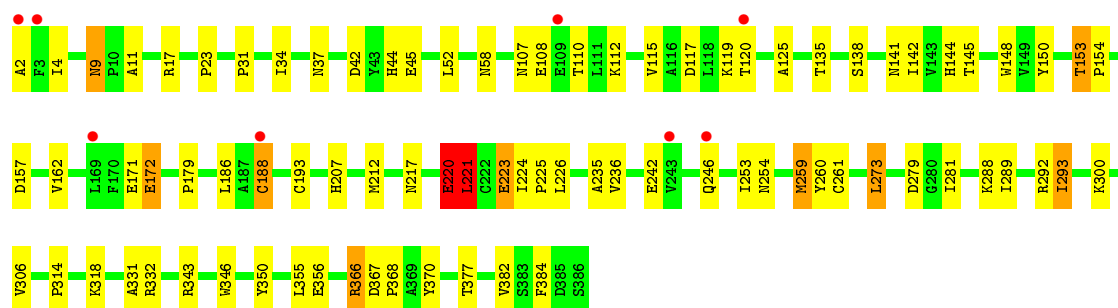
#### • Molecule 1: Sulfite reductase subunit alpha



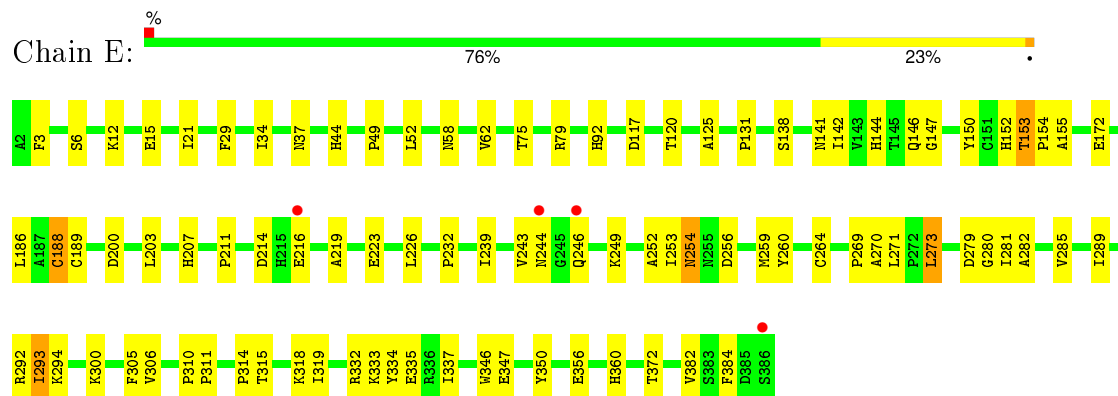
#### • Molecule 2: Sulfite reductase subunit beta



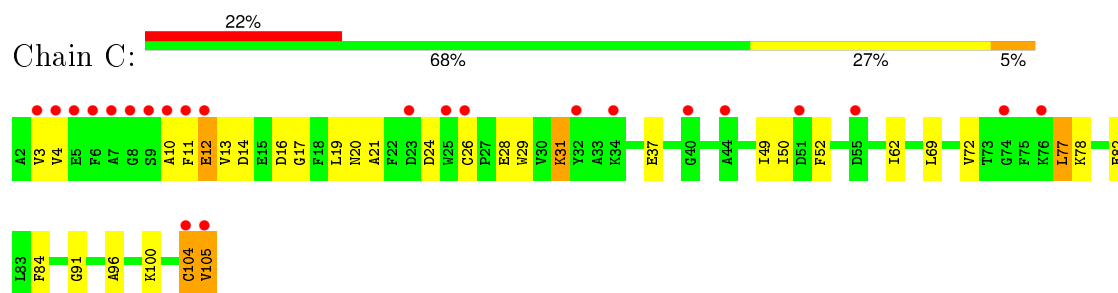




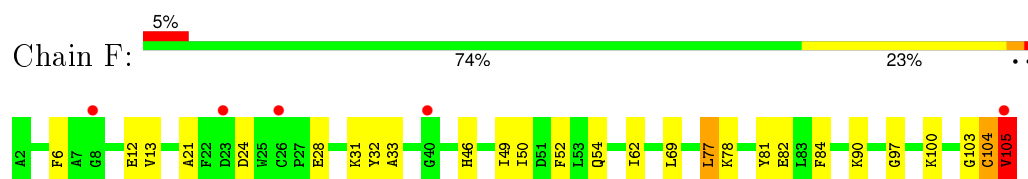
• Molecule 2: Sulfite reductase subunit beta



• Molecule 3: Sulfite reductase subunit gamma



• Molecule 3: Sulfite reductase subunit gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.13Å 59.98Å 133.21Å 90.00° 94.24° 90.00°	Depositor
Resolution (Å)	30.00 – 2.05 27.33 – 2.04	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.05) 96.9 (27.33-2.04)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 2.04Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.191 , 0.219 0.197 , 0.198	Depositor DCC
$R_{free}$ test set	5588 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.1	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 112112 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15433	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SF4, SO3, 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	0.65	9/3511 (0.3%)	0.72	1/4751 (0.0%)
1	D	0.73	10/3511 (0.3%)	0.76	5/4751 (0.1%)
2	B	0.80	15/3081 (0.5%)	0.76	6/4178 (0.1%)
2	E	0.48	5/3075 (0.2%)	0.64	0/4170
3	C	0.86	3/817 (0.4%)	0.84	4/1101 (0.4%)
3	F	0.64	3/811 (0.4%)	0.69	1/1093 (0.1%)
All	All	0.69	45/14806 (0.3%)	0.73	17/20044 (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	D	0	1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	220	GLU	CB-CG	-19.85	1.14	1.52
1	D	360	GLU	CD-OE1	-15.05	1.09	1.25
1	D	230	ALA	CA-CB	-14.84	1.21	1.52
2	B	220	GLU	CD-OE1	-12.16	1.12	1.25
1	D	360	GLU	CD-OE2	-11.52	1.12	1.25
2	B	223	GLU	CD-OE2	-9.88	1.14	1.25
3	C	104[A]	CYS	CB-SG	9.40	1.98	1.82
3	C	104[B]	CYS	CB-SG	9.40	1.98	1.82
1	D	393	GLU	CD-OE1	-9.01	1.15	1.25
2	B	220	GLU	CG-CD	-8.90	1.38	1.51
1	A	36	LYS	CB-CG	-8.89	1.28	1.52
1	D	393	GLU	CB-CG	-7.68	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	172	GLU	CB-CG	-7.62	1.37	1.52
3	F	105	VAL	CB-CG1	-7.62	1.36	1.52
1	A	341	MET	CG-SD	-7.39	1.61	1.81
1	D	393	GLU	CD-OE2	-7.29	1.17	1.25
1	D	87	GLN	CB-CG	-6.92	1.33	1.52
3	C	105	VAL	C-OXT	6.65	1.35	1.23
2	B	235	ALA	C-O	-5.95	1.12	1.23
1	A	334	PRO	CB-CG	-5.91	1.20	1.50
2	B	221	LEU	CG-CD2	-5.89	1.30	1.51
2	E	282	ALA	C-N	-5.86	1.20	1.34
3	F	13	VAL	C-N	-5.82	1.20	1.34
2	E	141	ASN	C-N	-5.79	1.20	1.34
1	A	87	GLN	C-N	-5.76	1.23	1.34
2	B	17	ARG	C-N	-5.63	1.21	1.34
2	E	49	PRO	C-O	-5.62	1.12	1.23
1	A	381	GLU	C-O	-5.51	1.12	1.23
1	D	87	GLN	C-O	-5.51	1.12	1.23
2	E	3	PHE	C-N	-5.48	1.21	1.34
1	A	245	LYS	C-N	-5.47	1.21	1.34
2	E	49	PRO	N-CD	-5.46	1.40	1.47
2	B	221	LEU	CG-CD1	-5.46	1.31	1.51
2	B	212	MET	C-N	-5.38	1.21	1.34
2	B	220	GLU	CD-OE2	-5.38	1.19	1.25
2	B	366	ARG	C-N	5.31	1.46	1.34
2	B	356	GLU	C-N	-5.31	1.21	1.34
1	D	298	ILE	C-N	-5.30	1.21	1.34
1	A	341	MET	CA-CB	-5.29	1.42	1.53
1	A	390	LYS	C-O	-5.29	1.13	1.23
1	D	309	CYS	C-N	-5.14	1.22	1.34
1	A	169	SER	C-O	-5.14	1.13	1.23
2	B	220	GLU	N-CA	-5.11	1.36	1.46
2	B	273	LEU	C-O	-5.10	1.13	1.23
3	F	97	GLY	C-N	-5.10	1.22	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	MET	CG-SD-CE	-13.98	77.83	100.20
3	C	104[A]	CYS	CB-CA-C	10.21	130.82	110.40
3	C	104[B]	CYS	CB-CA-C	10.21	130.82	110.40
1	D	336	LEU	CA-CB-CG	9.72	137.66	115.30
1	D	336	LEU	CB-CG-CD2	8.53	125.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	105	VAL	CG1-CB-CG2	8.10	123.87	110.90
2	B	188[A]	CYS	CA-CB-SG	-7.34	100.80	114.00
2	B	188[B]	CYS	CA-CB-SG	-7.34	100.80	114.00
1	D	228	SER	O-C-N	-7.24	111.12	122.70
2	B	220	GLU	OE1-CD-OE2	7.08	131.80	123.30
2	B	220	GLU	CG-CD-OE1	-6.95	104.41	118.30
2	B	355	LEU	O-C-N	-6.55	112.21	122.70
3	C	31	LYS	CD-CE-NZ	5.61	124.61	111.70
2	B	145	THR	O-C-N	-5.44	113.99	122.70
1	D	62	GLU	O-C-N	-5.20	114.38	122.70
1	D	134	GLY	N-CA-C	-5.08	100.40	113.10
3	F	33	ALA	O-C-N	-5.03	114.66	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	229	MET	Mainchain

## 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	3421	0	3274	122	0
1	D	3421	0	3274	125	0
2	B	3001	0	2968	83	0
2	E	2998	0	2963	83	0
3	C	793	0	776	33	0
3	F	790	0	769	30	0
4	A	16	0	0	1	0
4	B	15	0	0	2	0
4	D	16	0	0	1	0
4	E	15	0	0	0	0
5	A	8	0	0	2	0
5	D	8	0	0	0	0
6	A	63	0	34	9	0
6	B	62	0	34	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	63	0	34	15	0
6	E	62	0	34	4	0
7	A	157	0	0	2	0
7	B	139	0	0	4	0
7	C	8	0	0	0	0
7	D	212	0	0	2	0
7	E	149	0	0	2	0
7	F	16	0	0	1	0
All	All	15433	0	14160	401	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 14.

All (401) 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)
6:D:584:SRM:HH A	3:F:104:CYS:SG	1.48	1.54
2:B:188[B]:CYS:SG	4:B:803:SF4:S1	2.38	1.21
6:D:584:SRM:CHA	3:F:104:CYS:SG	2.28	1.19
1:D:170:ASN:HD22	1:D:208:PRO:HG3	1.21	1.04
1:D:167:SER:HB2	3:F:105:VAL:HG11	1.39	1.01
1:A:416:LYS:HB3	1:A:418:GLU:OE1	1.60	0.99
1:D:402:GLN:H	1:D:402:GLN:HE21	1.17	0.93
2:E:239:ILE:HD13	2:E:252:ALA:HB2	1.50	0.92
1:D:131:ASN:HB2	1:D:140:VAL:HB	1.53	0.89
1:A:136:THR:H	6:A:582:SRM:HBB2	1.40	0.87
1:A:290:THR:HB	1:A:297:SER:OG	1.73	0.86
1:A:308:HIS:HD2	2:B:292:ARG:HE	1.21	0.86
1:A:230:ALA:HB2	2:B:289:ILE:HD13	1.55	0.86
1:A:131:ASN:HB2	1:A:140:VAL:HB	1.59	0.84
1:D:104:GLN:NE2	1:D:104:GLN:H	1.76	0.83
1:D:136:THR:H	6:D:584:SRM:HBB2	1.43	0.82
2:E:223:GLU:OE1	2:E:226:LEU:HD11	1.80	0.82
2:E:37:ASN:HD21	2:E:58:ASN:HD21	1.27	0.82
1:D:170:ASN:ND2	1:D:208:PRO:HG3	1.95	0.81
5:A:6573:SO3:O1	3:C:100:LYS:NZ	2.14	0.80
1:D:104:GLN:HE21	1:D:104:GLN:H	1.30	0.79
1:A:416:LYS:CB	1:A:418:GLU:OE1	2.31	0.79
1:D:170:ASN:HB3	1:D:208:PRO:HA	1.64	0.79
2:E:314:PRO:O	2:E:318:LYS:HG3	1.84	0.77
2:E:219:ALA:HB2	2:E:249:LYS:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:ARG:C	2:B:368:PRO:HD2	2.06	0.76
1:A:170:ASN:ND2	1:A:208:PRO:HG3	2.00	0.76
3:C:3:VAL:HG22	3:C:12:GLU:OE2	1.86	0.76
1:A:104:GLN:H	1:A:104:GLN:NE2	1.84	0.75
2:E:117:ASP:O	2:E:120:THR:HG22	1.87	0.75
1:A:402:GLN:HE21	1:A:402:GLN:H	1.31	0.75
1:D:167:SER:CB	3:F:105:VAL:HG11	2.15	0.75
1:A:246:ILE:HG12	1:A:317:LEU:CD2	2.17	0.74
1:A:104:GLN:HE21	1:A:104:GLN:H	1.33	0.74
2:B:224:ILE:HB	2:B:225:PRO:HD3	1.70	0.74
1:A:229:MET:HG3	2:B:289:ILE:HD11	1.68	0.74
1:D:184:GLU:OE1	2:E:44:HIS:HD2	1.70	0.74
1:D:112:ALA:O	1:D:116:GLU:HG3	1.88	0.74
1:A:135:SER:HB2	6:A:582:SRM:HHC	1.70	0.73
1:A:133:HIS:HA	1:A:138:ASP:O	1.88	0.73
1:A:263:ALA:HB1	2:B:45:GLU:HA	1.72	0.72
1:D:97:PHE:O	2:E:150:TYR:HE1	1.72	0.72
1:A:39:ASP:OD1	2:B:2:ALA:HA	1.88	0.71
1:A:285:PRO:HG3	2:B:293:ILE:HA	1.72	0.71
2:B:332:ARG:HG3	2:B:343:ARG:NH2	2.05	0.71
2:B:37:ASN:HD21	2:B:58:ASN:HD21	1.39	0.71
1:A:427:ASP:OD2	1:A:429:SER:HB3	1.90	0.71
2:B:367:ASP:N	2:B:368:PRO:HD2	2.06	0.71
1:D:97:PHE:O	2:E:150:TYR:CE1	2.43	0.71
1:D:336:LEU:HD23	2:E:232:PRO:HG3	1.73	0.70
1:D:308:HIS:HD2	2:E:292:ARG:HE	1.39	0.70
1:A:196:GLN:HE22	1:A:354:PRO:HA	1.56	0.70
1:A:168:GLY:N	3:C:105:VAL:HG21	2.05	0.70
2:E:125:ALA:HB3	7:E:400:HOH:O	1.90	0.70
2:B:382:VAL:CG2	2:B:384:PHE:HD2	2.05	0.69
3:F:78:LYS:O	3:F:82:GLU:HG3	1.92	0.69
1:D:402:GLN:H	1:D:402:GLN:NE2	1.89	0.69
1:D:416:LYS:O	1:D:419:GLU:HG2	1.93	0.68
1:A:46:CYS:HB3	1:A:47:PRO:HD3	1.75	0.68
1:D:223:ASN:HD21	1:D:311:ASN:HD21	1.38	0.68
1:A:34:ASN:HD21	1:A:38:LEU:H	1.41	0.68
1:A:408:ARG:HH11	1:A:410:ASN:HD21	1.39	0.68
1:D:262:ASN:ND2	2:E:292:ARG:HH22	1.92	0.68
1:A:124:LEU:HD21	2:B:4:ILE:HD11	1.76	0.68
2:B:350:TYR:HB3	2:B:384:PHE:HZ	1.58	0.67
1:D:104:GLN:HE22	1:D:173:THR:HG21	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:ARG:HH11	1:D:410:ASN:HD21	1.41	0.67
1:A:136:THR:H	6:A:582:SRM:CBB	2.07	0.67
1:A:168:GLY:HA2	3:C:105:VAL:HB	1.76	0.67
3:C:12:GLU:HB3	3:C:20:ASN:HD22	1.60	0.67
3:C:49:ILE:HD12	3:C:84:PHE:HE1	1.60	0.67
6:D:584:SRM:HDA2	3:F:104:CYS:SG	2.35	0.67
1:D:89:GLU:H	1:D:89:GLU:CD	1.98	0.66
1:A:262:ASN:ND2	2:B:292:ARG:HH22	1.94	0.66
1:A:170:ASN:HB2	1:A:204:GLU:O	1.95	0.66
1:A:219:ASP:OD1	1:A:226:VAL:HG12	1.95	0.66
6:D:584:SRM:HMA2	3:F:104:CYS:HB3	1.78	0.65
1:D:336:LEU:CD2	2:E:232:PRO:HG3	2.26	0.65
1:D:136:THR:H	6:D:584:SRM:CBB	2.09	0.65
1:D:34:ASN:HD21	1:D:38:LEU:H	1.45	0.65
2:B:223:GLU:HB2	2:B:226:LEU:HD12	1.79	0.65
1:D:246:ILE:HG12	1:D:317:LEU:CD1	2.27	0.65
1:D:121:VAL:HG13	1:D:155:GLU:OE1	1.98	0.64
2:E:223:GLU:OE1	2:E:226:LEU:CD1	2.45	0.64
3:F:28:GLU:HA	3:F:31:LYS:HE2	1.78	0.64
1:A:410:ASN:HD22	1:A:412:TYR:H	1.44	0.64
1:D:33:LYS:HE3	1:D:35:PRO:HG3	1.79	0.64
1:A:170:ASN:HD22	1:A:208:PRO:HG3	1.62	0.64
1:D:434:ARG:HB2	1:D:434:ARG:NH1	2.13	0.64
2:B:37:ASN:HD21	2:B:58:ASN:ND2	1.96	0.64
1:A:402:GLN:NE2	1:A:402:GLN:H	1.95	0.64
2:E:281:ILE:O	2:E:306:VAL:HG22	1.98	0.64
2:B:281:ILE:O	2:B:306:VAL:HG22	1.98	0.63
6:D:584:SRM:O1A	2:E:150:TYR:HD2	1.80	0.63
1:D:155:GLU:HG3	2:E:6:SER:HB2	1.80	0.63
6:D:584:SRM:HMA2	3:F:104:CYS:CB	2.29	0.63
1:A:97:PHE:O	2:B:150:TYR:CE1	2.52	0.63
1:A:223:ASN:HD21	1:A:311:ASN:HD21	1.44	0.63
1:D:196:GLN:HE22	1:D:354:PRO:HA	1.64	0.62
2:E:223:GLU:HB3	3:F:62:ILE:HG22	1.81	0.62
2:B:107:ASN:ND2	2:B:110:THR:H	1.97	0.62
3:C:4:VAL:O	3:C:10:ALA:HA	2.00	0.62
1:D:168:GLY:N	3:F:105:VAL:HG13	2.15	0.61
2:E:223:GLU:HB2	2:E:226:LEU:HD12	1.81	0.61
1:D:434:ARG:HB2	1:D:434:ARG:HH11	1.64	0.61
1:D:313:MET:HB2	1:D:317:LEU:HD23	1.81	0.61
2:E:243:VAL:HG12	2:E:244:ASN:ND2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ARG:H	1:D:98:HIS:HD2	1.49	0.61
1:A:83:ARG:H	1:A:98:HIS:HD2	1.49	0.61
1:A:418:GLU:H	1:A:418:GLU:CD	2.05	0.61
1:A:418:GLU:N	1:A:418:GLU:OE2	2.30	0.61
1:D:410:ASN:HD22	1:D:412:TYR:H	1.49	0.61
1:A:436:MET:SD	1:D:89:GLU:OE1	2.59	0.60
1:D:104:GLN:N	1:D:104:GLN:HE21	1.98	0.60
1:D:98:HIS:HE1	1:D:146:THR:OG1	1.83	0.60
1:D:317:LEU:N	1:D:317:LEU:HD22	2.16	0.60
1:D:167:SER:OG	3:F:105:VAL:HG21	2.01	0.60
2:E:146:GLN:HE21	2:E:150:TYR:HB3	1.65	0.60
1:A:104:GLN:HE22	1:A:173:THR:HG21	1.66	0.60
1:A:184:GLU:OE1	2:B:44:HIS:HD2	1.85	0.60
2:B:350:TYR:HB3	2:B:384:PHE:CZ	2.37	0.60
2:E:356:GLU:OE2	2:E:356:GLU:HA	2.01	0.60
2:E:315:THR:O	2:E:319:ILE:HG13	2.02	0.59
1:A:308:HIS:CD2	2:B:292:ARG:HE	2.11	0.59
2:B:382:VAL:HG22	1:D:402:GLN:OE1	2.03	0.59
2:B:153:THR:N	2:B:154:PRO:CD	2.66	0.59
1:D:248:GLN:HE22	1:D:296:LEU:H	1.49	0.59
1:A:402:GLN:OE1	2:E:382:VAL:HG22	2.02	0.59
3:C:26:CYS:SG	3:C:28:GLU:HG2	2.42	0.59
1:D:168:GLY:H	3:F:105:VAL:HG13	1.68	0.59
3:F:21:ALA:HB3	3:F:24:ASP:OD2	2.02	0.59
1:D:402:GLN:HE21	1:D:402:GLN:N	1.97	0.58
1:D:229:MET:HG3	2:E:289:ILE:HD11	1.86	0.58
1:A:97:PHE:O	2:B:150:TYR:HE1	1.86	0.58
1:D:220:GLY:HA3	4:D:806:SF4:S4	2.43	0.58
2:B:223:GLU:HG2	3:C:62:ILE:HA	1.84	0.57
1:D:170:ASN:HB2	1:D:204:GLU:O	2.05	0.57
2:B:188[B]:CYS:SG	4:B:803:SF4:S2	3.03	0.57
1:D:416:LYS:HB3	1:D:418:GLU:OE2	2.05	0.57
1:A:70:ILE:HG13	3:C:100:LYS:HG3	1.85	0.57
1:D:42:ILE:HD11	1:D:126:GLY:C	2.25	0.57
1:A:168:GLY:H	3:C:105:VAL:HG21	1.70	0.57
1:A:318:LYS:HE3	2:B:42:ASP:O	2.04	0.57
2:B:207:HIS:HD2	2:B:279:ASP:OD1	1.88	0.56
1:D:306:CYS:O	1:D:307:MET:HB2	2.04	0.56
2:B:236:VAL:HG22	2:B:253:ILE:HG12	1.88	0.56
1:A:406:GLU:HG3	2:E:346:TRP:HE1	1.70	0.56
3:C:104[B]:CYS:HB3	3:C:105:VAL:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ILE:HD11	1:A:126:GLY:C	2.26	0.56
6:A:582:SRM:O1A	2:B:150:TYR:HD2	1.89	0.56
2:B:186:LEU:C	2:B:186:LEU:HD23	2.25	0.56
1:A:416:LYS:HE3	1:A:418:GLU:OE1	2.06	0.56
3:C:52:PHE:CE1	3:C:72:VAL:HG11	2.42	0.55
2:E:280:GLY:HA3	2:E:305:PHE:CE1	2.41	0.55
2:B:242:GLU:HA	2:B:246:GLN:O	2.06	0.55
2:B:382:VAL:HG21	2:B:384:PHE:HD2	1.70	0.55
1:D:308:HIS:CD2	2:E:292:ARG:HE	2.22	0.55
2:E:211:PRO:HG2	2:E:253:ILE:CD1	2.37	0.55
6:D:584:SRM:CED	3:F:104:CYS:SG	2.95	0.54
1:A:246:ILE:HD11	1:A:298:ILE:HD12	1.87	0.54
1:D:34:ASN:N	1:D:35:PRO:HD3	2.22	0.54
2:E:306:VAL:HG11	2:E:319:ILE:HD12	1.89	0.54
1:A:335:VAL:HG12	7:B:405:HOH:O	2.07	0.54
1:D:230:ALA:HB2	2:E:289:ILE:HD13	1.90	0.54
1:A:229:MET:CG	2:B:289:ILE:HD11	2.37	0.54
1:D:246:ILE:HG12	1:D:317:LEU:HD13	1.88	0.54
2:B:31:PRO:HG2	2:B:34:ILE:CG1	2.38	0.54
1:D:202:GLN:OE1	1:D:206:HIS:HE1	1.90	0.54
2:B:224:ILE:HD13	7:B:451:HOH:O	2.07	0.54
2:B:9:ASN:ND2	2:B:11:ALA:H	2.05	0.54
1:A:8:MET:HE3	1:A:59:HIS:HA	1.88	0.54
1:A:69:GLY:O	1:A:70:ILE:HD13	2.07	0.54
2:B:367:ASP:N	2:B:368:PRO:CD	2.70	0.54
1:A:245:LYS:HB2	1:A:318:LYS:HB2	1.89	0.54
1:A:427:ASP:CG	1:A:429:SER:HB3	2.27	0.54
1:A:104:GLN:HE21	1:A:104:GLN:N	2.05	0.54
1:D:418:GLU:H	1:D:418:GLU:CD	2.11	0.54
1:D:17:TRP:CD2	1:D:18:PRO:HD2	2.43	0.54
1:D:55:GLU:OE2	1:D:59:HIS:HE1	1.91	0.54
2:B:300:LYS:CB	1:D:407:PRO:HG2	2.39	0.54
1:D:133:HIS:HA	1:D:138:ASP:O	2.07	0.53
2:B:289:ILE:HG22	6:B:581:SRM:CCC	2.37	0.53
1:D:131:ASN:HB2	1:D:140:VAL:CB	2.31	0.53
2:E:211:PRO:HG2	2:E:253:ILE:HD13	1.90	0.53
1:A:306:CYS:O	1:A:307:MET:HB2	2.09	0.53
1:A:435:HIS:HE1	1:D:62:GLU:OE2	1.92	0.53
2:E:254:ASN:ND2	2:E:256:ASP:H	2.07	0.53
2:B:300:LYS:HB3	1:D:407:PRO:HG2	1.90	0.53
1:D:4:HIS:N	1:D:5:PRO:HD2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:THR:N	2:B:150:TYR:OH	2.42	0.53
1:D:42:ILE:HD11	1:D:126:GLY:O	2.09	0.53
2:E:153:THR:N	2:E:154:PRO:CD	2.72	0.52
1:D:136:THR:OG1	6:D:584:SRM:HBB1	2.10	0.52
1:A:98:HIS:HE1	1:A:146:THR:OG1	1.92	0.52
2:B:9:ASN:HD21	2:B:11:ALA:HB3	1.75	0.52
2:E:211:PRO:HA	2:E:273:LEU:HB3	1.91	0.52
3:C:21:ALA:HB3	3:C:24:ASP:OD2	2.09	0.52
3:F:105:VAL:CG2	3:F:105:VAL:OXT	2.58	0.52
1:A:70:ILE:HG12	3:C:100:LYS:HD2	1.91	0.52
1:D:56:LEU:HD13	1:D:64:HIS:CE1	2.45	0.51
1:D:76:TYR:CD1	1:D:206:HIS:HB3	2.46	0.51
3:F:77:LEU:HD22	3:F:81:TYR:CE1	2.46	0.51
2:B:142:ILE:O	2:B:144:HIS:HD2	1.94	0.51
2:E:246:GLN:OE1	2:E:246:GLN:HA	2.11	0.51
1:A:124:LEU:HD21	2:B:4:ILE:CD1	2.40	0.51
1:A:146:THR:HB	1:A:147:PRO:HD3	1.92	0.50
2:E:152:HIS:C	2:E:154:PRO:HD2	2.31	0.50
1:D:170:ASN:HD22	1:D:208:PRO:CG	2.10	0.50
2:E:153:THR:N	2:E:154:PRO:HD2	2.26	0.50
1:D:209:ALA:HB2	3:F:77:LEU:HD12	1.94	0.50
1:A:220:GLY:HA3	4:A:802:SF4:S1	2.51	0.50
1:A:103:ALA:HB1	2:B:23:PRO:HB3	1.93	0.50
1:A:363:GLU:O	1:A:367:GLU:HG3	2.11	0.50
1:A:196:GLN:HE22	1:A:354:PRO:CA	2.25	0.50
1:D:46:CYS:HB3	1:D:47:PRO:HD3	1.93	0.50
3:C:11:PHE:CE2	3:C:29:TRP:HB2	2.47	0.50
2:E:37:ASN:HD21	2:E:58:ASN:ND2	2.02	0.50
1:A:136:THR:OG1	6:A:582:SRM:HBB1	2.12	0.49
1:A:36:LYS:HB2	7:A:506:HOH:O	2.10	0.49
2:B:370:TYR:CE1	1:D:340:GLN:HG2	2.47	0.49
1:A:205:LEU:O	1:A:205:LEU:HD23	2.12	0.49
2:E:207:HIS:HD2	2:E:279:ASP:OD1	1.94	0.49
1:A:50:LEU:HD13	1:A:50:LEU:C	2.33	0.49
2:E:382:VAL:CG2	2:E:384:PHE:HD1	2.26	0.49
1:D:316:ALA:C	1:D:317:LEU:HD22	2.33	0.49
2:B:223:GLU:OE1	2:B:226:LEU:HD11	2.12	0.49
1:D:83:ARG:H	1:D:98:HIS:CD2	2.31	0.49
1:A:131:ASN:HB2	1:A:140:VAL:CB	2.37	0.49
2:B:52:LEU:HD21	6:B:581:SRM:CCA	2.43	0.49
1:D:8:MET:CE	2:E:311:PRO:HD3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HB3	1:A:139:ILE:HB	1.93	0.49
2:B:217:ASN:ND2	1:D:437:ARG:NH1	2.60	0.48
1:A:17:TRP:CD2	1:A:18:PRO:HD2	2.47	0.48
3:C:11:PHE:HE2	3:C:26:CYS:HG	1.60	0.48
2:B:289:ILE:HG22	6:B:581:SRM:O2C	2.12	0.48
1:D:3:LYS:N	1:D:3:LYS:HD3	2.28	0.48
3:C:78:LYS:O	3:C:82:GLU:HG3	2.12	0.48
1:A:79:GLY:H	1:A:167:SER:HG	1.60	0.48
2:B:382:VAL:HG21	2:B:384:PHE:CD2	2.47	0.48
1:D:104:GLN:N	1:D:104:GLN:NE2	2.55	0.48
6:A:582:SRM:HMA2	3:C:104[B]:CYS:HA	1.96	0.48
1:D:8:MET:HE2	2:E:311:PRO:HD3	1.95	0.48
3:F:50:ILE:O	3:F:54:GLN:HG3	2.14	0.48
1:D:135:SER:HB2	6:D:584:SRM:HHC	1.96	0.48
1:A:170:ASN:HD22	1:A:208:PRO:CG	2.27	0.48
2:B:31:PRO:HG2	2:B:34:ILE:HG12	1.95	0.47
2:E:186:LEU:HD23	2:E:186:LEU:C	2.34	0.47
2:B:179:PRO:HG2	2:B:331:ALA:HB3	1.95	0.47
1:D:225:CYS:SG	6:E:583:SRM:NC	2.87	0.47
2:E:293:ILE:HG22	2:E:294:LYS:CD	2.44	0.47
2:E:293:ILE:HG22	2:E:294:LYS:HD3	1.96	0.47
1:D:60:GLU:OE1	1:D:64:HIS:CE1	2.68	0.47
2:E:138:SER:HB2	2:E:172:GLU:O	2.15	0.47
3:C:37:GLU:OE1	3:C:91:GLY:HA2	2.15	0.47
1:D:20:PHE:O	1:D:24:ILE:HG13	2.15	0.47
6:D:584:SRM:HHB	6:D:584:SRM:HBA1	1.96	0.47
1:D:102:LEU:HB3	1:D:139:ILE:HB	1.95	0.47
2:B:220:GLU:H	2:B:220:GLU:HG2	1.57	0.47
3:F:46:HIS:O	3:F:50:ILE:HG12	2.14	0.47
1:D:111:THR:HG23	2:E:29:PHE:HD2	1.80	0.47
1:A:428:ILE:CD1	2:E:214:ASP:HB2	2.45	0.47
3:C:13:VAL:HG12	3:C:14:ASP:N	2.30	0.46
1:D:237:ILE:HD12	1:D:328:LEU:HD13	1.96	0.46
2:E:254:ASN:HD22	2:E:254:ASN:C	2.19	0.46
2:E:200:ASP:O	2:E:285:VAL:HA	2.15	0.46
2:E:52:LEU:HD21	6:E:583:SRM:O2A	2.15	0.46
1:D:262:ASN:HD21	2:E:292:ARG:HH12	1.64	0.46
1:A:42:ILE:HD11	1:A:126:GLY:O	2.15	0.46
1:A:28:CYS:SG	1:A:47:PRO:HB2	2.56	0.46
1:D:317:LEU:CD2	1:D:317:LEU:N	2.77	0.46
2:B:107:ASN:HD21	2:B:110:THR:H	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:LYS:HB2	1:D:232:SER:HB3	1.98	0.46
2:E:270:ALA:O	2:E:271:LEU:HD12	2.15	0.46
1:D:50:LEU:C	1:D:50:LEU:HD13	2.36	0.45
1:D:67:HIS:CG	2:E:269:PRO:HB3	2.51	0.45
2:E:216:GLU:HA	2:E:243:VAL:HG21	1.99	0.45
1:A:202:GLN:OE1	1:A:206:HIS:HE1	2.00	0.45
1:D:335:VAL:HA	1:D:336:LEU:HA	1.69	0.45
2:B:300:LYS:HE2	1:D:406:GLU:OE1	2.16	0.45
1:A:86:ASP:OD2	1:D:435:HIS:HD2	1.99	0.45
3:C:49:ILE:HG23	3:C:69:LEU:HD11	1.98	0.45
1:D:434:ARG:HH11	1:D:434:ARG:CB	2.29	0.45
2:B:108:GLU:O	2:B:112:LYS:HG3	2.17	0.45
2:B:148:TRP:CE3	2:B:157:ASP:HB2	2.51	0.45
1:A:225:CYS:SG	6:B:581:SRM:NC	2.90	0.45
1:A:406:GLU:HG2	2:E:300:LYS:HE2	1.99	0.45
6:D:584:SRM:HMA2	3:F:104:CYS:SG	2.57	0.44
2:B:382:VAL:CG2	2:B:384:PHE:CD2	2.95	0.44
1:D:279:GLU:O	1:D:308:HIS:HE1	1.99	0.44
2:B:153:THR:N	2:B:154:PRO:HD2	2.31	0.44
2:B:9:ASN:C	2:B:9:ASN:HD22	2.20	0.44
1:A:121:VAL:HG13	1:A:155:GLU:OE1	2.17	0.44
6:B:581:SRM:HBA1	6:B:581:SRM:HMA3	1.99	0.44
1:A:246:ILE:HG12	1:A:317:LEU:HD23	1.97	0.44
2:B:138:SER:HB2	2:B:172:GLU:O	2.17	0.44
6:D:584:SRM:C1A	3:F:104:CYS:SG	3.00	0.44
1:A:430:ASP:O	1:A:433:LYS:HB3	2.17	0.44
2:E:200:ASP:HB3	2:E:337:ILE:HD12	1.99	0.44
1:D:13:GLU:HB3	2:E:125:ALA:CB	2.47	0.44
1:A:427:ASP:OD1	1:A:429:SER:HB3	2.18	0.44
1:A:62:GLU:OE1	1:D:435:HIS:HE1	2.00	0.44
2:B:259:MET:SD	2:B:261:CYS:HB3	2.57	0.44
2:E:332:ARG:O	2:E:335:GLU:HB2	2.17	0.44
3:F:77:LEU:HD22	3:F:81:TYR:HE1	1.82	0.44
1:A:340:GLN:OE1	1:A:384:LYS:HD2	2.18	0.44
6:D:584:SRM:O1A	2:E:150:TYR:CD2	2.65	0.44
1:A:122:TRP:O	1:A:126:GLY:N	2.49	0.44
1:A:205:LEU:C	1:A:205:LEU:HD23	2.38	0.44
2:E:29:PHE:O	2:E:92:HIS:HD2	2.00	0.44
3:F:49:ILE:HD12	3:F:84:PHE:HE1	1.80	0.44
1:D:8:MET:HE2	2:E:310:PRO:C	2.38	0.44
1:D:427:ASP:OD2	1:D:429:SER:OG	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:PRO:HG3	7:D:504:HOH:O	2.18	0.44
1:A:284:CYS:HA	1:A:285:PRO:HD3	1.89	0.43
1:A:406:GLU:O	2:E:372:THR:HB	2.18	0.43
1:D:31:ARG:HD3	1:D:47:PRO:HG2	2.01	0.43
3:C:13:VAL:HG11	3:C:17:GLY:HA2	1.99	0.43
2:B:125:ALA:HB3	7:B:407:HOH:O	2.18	0.43
1:D:219:ASP:OD1	1:D:226:VAL:HG12	2.17	0.43
1:D:87:GLN:N	1:D:88:PRO:HD3	2.33	0.43
1:A:209:ALA:HB2	3:C:77:LEU:CD1	2.49	0.43
3:F:6:PHE:CD2	3:F:32:TYR:HB2	2.53	0.43
3:C:50:ILE:HG23	3:C:96:ALA:HA	2.00	0.43
1:D:130:THR:HB	1:D:140:VAL:O	2.18	0.43
1:A:225:CYS:HA	6:B:581:SRM:C1C	2.49	0.43
2:B:366:ARG:CB	2:B:368:PRO:HD2	2.49	0.43
1:A:113:GLU:HG3	7:A:484:HOH:O	2.18	0.43
1:D:181:SER:O	2:E:34:ILE:HG23	2.19	0.43
1:A:410:ASN:ND2	1:A:410:ASN:C	2.72	0.43
1:A:106:ALA:O	1:A:107:ALA:HB3	2.19	0.43
6:A:582:SRM:O1A	2:B:150:TYR:CD2	2.71	0.43
1:D:34:ASN:HD21	1:D:38:LEU:N	2.15	0.43
1:D:121:VAL:HG11	1:D:156:MET:HE2	2.00	0.43
1:A:209:ALA:HB2	3:C:77:LEU:HD12	2.00	0.43
1:A:167:SER:C	3:C:105:VAL:HG11	2.39	0.43
1:D:3:LYS:HB2	1:D:4:HIS:H	1.58	0.42
1:D:252:LYS:HE2	7:D:632:HOH:O	2.19	0.42
1:A:312:THR:C	1:A:314:PRO:HD3	2.39	0.42
6:A:582:SRM:HHB	6:A:582:SRM:HBA1	2.01	0.42
1:A:202:GLN:OE1	1:A:206:HIS:CE1	2.73	0.42
1:D:70:ILE:HG13	3:F:100:LYS:HG3	2.01	0.42
2:B:171:GLU:HA	2:B:171:GLU:OE1	2.19	0.42
6:E:583:SRM:HMA3	6:E:583:SRM:HBA1	2.02	0.42
2:B:288:LYS:NZ	7:B:402:HOH:O	2.51	0.42
2:E:12:LYS:HD3	2:E:15:GLU:OE2	2.20	0.42
2:B:52:LEU:CD1	2:B:135:THR:HG21	2.48	0.42
2:E:350:TYR:HB3	2:E:384:PHE:CZ	2.54	0.42
1:A:9:LEU:HD21	1:A:54:LEU:HD13	2.02	0.42
2:E:37:ASN:ND2	2:E:58:ASN:HD21	2.06	0.42
5:A:6573:SO3:S	3:C:100:LYS:NZ	2.91	0.42
6:A:582:SRM:C4C	2:B:193:CYS:HA	2.49	0.42
2:E:264:CYS:SG	2:E:271:LEU:HD23	2.60	0.42
2:E:75:THR:O	2:E:79:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ASN:HD22	2:E:21:ILE:HD12	1.84	0.42
2:B:115:VAL:CG1	2:B:119:LYS:HE3	2.50	0.42
1:D:168:GLY:CA	3:F:105:VAL:HG22	2.50	0.41
1:A:308:HIS:HD2	2:B:292:ARG:NE	2.02	0.41
1:A:188:TYR:OH	1:A:218:PHE:HB3	2.20	0.41
1:A:419:GLU:OE2	2:E:360:HIS:HE1	2.04	0.41
2:B:223:GLU:O	2:B:224:ILE:C	2.57	0.41
3:F:52:PHE:CD2	3:F:69:LEU:HD12	2.54	0.41
2:E:62:VAL:O	2:E:62:VAL:HG13	2.20	0.41
1:A:400:VAL:HG22	1:A:403:HIS:CE1	2.54	0.41
3:F:90:LYS:HE2	7:F:642:HOH:O	2.19	0.41
1:A:99:THR:HG23	1:A:140:VAL:HG13	2.01	0.41
1:A:428:ILE:HD13	2:E:214:ASP:HB2	2.02	0.41
2:E:142:ILE:O	2:E:144:HIS:HD2	2.03	0.41
2:B:117:ASP:O	2:B:120:THR:OG1	2.30	0.41
2:E:147:GLY:N	2:E:188:CYS:SG	2.91	0.41
2:E:382:VAL:HG21	2:E:384:PHE:HD1	1.86	0.41
1:A:42:ILE:HG22	1:A:145:GLN:HG3	2.01	0.41
1:D:18:PRO:HD3	2:E:131:PRO:HG3	2.01	0.41
2:E:155:ALA:O	2:E:279:ASP:HB3	2.21	0.41
1:A:148:GLN:O	1:A:152:ILE:HG13	2.21	0.41
2:B:144:HIS:CG	2:B:162:VAL:HG21	2.55	0.41
2:E:347:GLU:HG2	7:E:392:HOH:O	2.21	0.41
2:B:346:TRP:CZ2	1:D:407:PRO:HD2	2.55	0.41
3:F:103:GLY:O	3:F:105:VAL:N	2.54	0.41
1:A:70:ILE:H	3:C:16:ASP:CG	2.24	0.41
1:A:410:ASN:HD22	1:A:410:ASN:C	2.24	0.41
1:D:33:LYS:HE3	1:D:33:LYS:HB3	1.87	0.41
1:A:83:ARG:H	1:A:98:HIS:CD2	2.33	0.41
3:C:19:LEU:HD21	3:C:29:TRP:CE3	2.56	0.41
1:D:225:CYS:HA	6:E:583:SRM:C1C	2.51	0.41
1:D:253:ALA:HB3	1:D:259:PHE:CD2	2.56	0.41
1:A:346:ILE:HG21	1:A:349:ILE:HB	2.02	0.41
1:A:168:GLY:CA	3:C:105:VAL:HB	2.45	0.41
2:B:217:ASN:O	2:B:221:LEU:HD22	2.20	0.41
1:A:193:MET:HA	1:A:355:PHE:CE1	2.56	0.41
1:D:333:ALA:HB1	1:D:334:PRO:HD2	2.03	0.40
1:D:13:GLU:HB3	2:E:125:ALA:HB1	2.03	0.40
1:A:171:LEU:O	1:A:205:LEU:HG	2.21	0.40
1:D:226:VAL:O	1:D:226:VAL:HG22	2.22	0.40
1:A:45:GLU:HA	1:A:48:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:THR:HG21	1:D:237:ILE:HG21	2.03	0.40
1:A:248:GLN:NE2	1:A:248:GLN:HA	2.36	0.40
1:D:331:ALA:HA	1:D:340:GLN:O	2.22	0.40
2:E:333:LYS:O	2:E:334:TYR:HB2	2.22	0.40
2:B:314:PRO:O	2:B:318:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/435 (100%)	412 (95%)	21 (5%)	0	100	100
1	D	433/435 (100%)	417 (96%)	15 (4%)	1 (0%)	52	43
2	B	384/385 (100%)	370 (96%)	11 (3%)	3 (1%)	24	12
2	E	383/385 (100%)	364 (95%)	17 (4%)	2 (0%)	34	22
3	C	103/104 (99%)	100 (97%)	3 (3%)	0	100	100
3	F	102/104 (98%)	98 (96%)	3 (3%)	1 (1%)	19	8
All	All	1838/1848 (100%)	1761 (96%)	70 (4%)	7 (0%)	39	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	141	ASN
3	F	104	CYS
2	B	293	ILE
1	D	133	HIS
2	E	153	THR
2	E	293	ILE
2	B	153	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	364/364 (100%)	351 (96%)	13 (4%)	42	34
1	D	364/364 (100%)	351 (96%)	13 (4%)	42	34
2	B	325/324 (100%)	318 (98%)	7 (2%)	60	53
2	E	324/324 (100%)	317 (98%)	7 (2%)	60	53
3	C	81/80 (101%)	78 (96%)	3 (4%)	41	32
3	F	80/80 (100%)	77 (96%)	3 (4%)	40	31
All	All	1538/1536 (100%)	1492 (97%)	46 (3%)	48	41

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	36	LYS
1	A	54	LEU
1	A	56	LEU
1	A	104	GLN
1	A	131	ASN
1	A	192	LEU
1	A	212	TYR
1	A	335	VAL
1	A	391	LEU
1	A	402	GLN
1	A	410	ASN
1	A	430	ASP
2	B	9	ASN
2	B	220	GLU
2	B	221	LEU
2	B	254	ASN
2	B	259	MET
2	B	260	TYR
2	B	273	LEU
3	C	12	GLU
3	C	31	LYS

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Mol	Chain	Res	Type
3	C	77	LEU
1	D	3	LYS
1	D	4	HIS
1	D	34	ASN
1	D	45	GLU
1	D	54	LEU
1	D	56	LEU
1	D	89	GLU
1	D	104	GLN
1	D	212	TYR
1	D	336	LEU
1	D	345	LEU
1	D	402	GLN
1	D	432	ARG
2	E	188	CYS
2	E	189	CYS
2	E	203	LEU
2	E	254	ASN
2	E	259	MET
2	E	260	TYR
2	E	273	LEU
3	F	12	GLU
3	F	77	LEU
3	F	105	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	64	HIS
1	A	67	HIS
1	A	98	HIS
1	A	104	GLN
1	A	159	ASN
1	A	161	ASN
1	A	170	ASN
1	A	196	GLN
1	A	206	HIS
1	A	248	GLN
1	A	262	ASN
1	A	308	HIS
1	A	311	ASN

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Mol	Chain	Res	Type
1	A	402	GLN
1	A	409	HIS
1	A	410	ASN
1	A	435	HIS
2	B	9	ASN
2	B	37	ASN
2	B	44	HIS
2	B	92	HIS
2	B	107	ASN
2	B	144	HIS
2	B	191	ASN
2	B	207	HIS
2	B	215	HIS
2	B	217	ASN
2	B	254	ASN
2	B	263	ASN
3	C	20	ASN
3	C	60	ASN
1	D	34	ASN
1	D	67	HIS
1	D	87	GLN
1	D	98	HIS
1	D	104	GLN
1	D	161	ASN
1	D	170	ASN
1	D	196	GLN
1	D	206	HIS
1	D	248	GLN
1	D	262	ASN
1	D	308	HIS
1	D	311	ASN
1	D	402	GLN
1	D	409	HIS
1	D	410	ASN
1	D	435	HIS
2	E	37	ASN
2	E	40	ASN
2	E	44	HIS
2	E	144	HIS
2	E	146	GLN
2	E	191	ASN
2	E	207	HIS

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Mol	Chain	Res	Type
2	E	215	HIS
2	E	244	ASN
2	E	254	ASN
2	E	263	ASN
2	E	360	HIS
3	F	47	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](#)

16 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	$\# Z  > 2$
6	SRM	A	582	2,5	29,70,70	1.60	5 (17%)	29,112,112	3.47	7 (24%)
5	SO3	A	6573	-	1,3,3	0.55	0	0,3,3	0.00	-
5	SO3	A	6574	6	1,3,3	1.16	0	0,3,3	0.00	-
4	SF4	A	801	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	A	802	1	0,12,12	0.00	-	0,24,24	0.00	-
6	SRM	B	581	-	28,66,70	1.42	4 (14%)	37,98,112	3.55	12 (32%)
4	SF4	B	803	2	0,9,12	0.00	-	0,15,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SF4	B	804	2	0,12,12	0.00	-	0,24,24	0.00	-
6	SRM	D	584	2,5	29,70,70	1.57	4 (13%)	29,112,112	3.47	7 (24%)
5	SO3	D	6575	-	1,3,3	0.53	0	0,3,3	0.00	-
5	SO3	D	6576	6	1,3,3	1.22	0	0,3,3	0.00	-
4	SF4	D	805	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	D	806	1	0,12,12	0.00	-	0,24,24	0.00	-
6	SRM	E	583	-	28,66,70	1.34	3 (10%)	37,98,112	3.56	14 (37%)
4	SF4	E	807	2	0,9,12	0.00	-	0,15,24	0.00	-
4	SF4	E	808	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
6	SRM	A	582	2,5	-	0/22/126/126	0/0/8/8
5	SO3	A	6573	-	-	0/0/0/0	0/0/0/0
5	SO3	A	6574	6	-	0/0/0/0	0/0/0/0
4	SF4	A	801	1	-	0/0/48/48	0/6/5/5
4	SF4	A	802	1	-	0/0/48/48	0/6/5/5
6	SRM	B	581	-	-	0/33/94/126	0/0/4/8
4	SF4	B	803	2	-	0/0/24/48	0/0/2/5
4	SF4	B	804	2	-	0/0/48/48	0/6/5/5
6	SRM	D	584	2,5	-	0/22/126/126	0/0/8/8
5	SO3	D	6575	-	-	0/0/0/0	0/0/0/0
5	SO3	D	6576	6	-	0/0/0/0	0/0/0/0
4	SF4	D	805	1	-	0/0/48/48	0/6/5/5
4	SF4	D	806	1	-	0/0/48/48	0/6/5/5
6	SRM	E	583	-	-	0/33/94/126	0/0/4/8
4	SF4	E	807	2	-	0/0/24/48	0/3/3/5
4	SF4	E	808	2	-	0/0/48/48	0/6/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	581	SRM	C1A-NA	2.28	1.40	1.37
6	E	583	SRM	C1A-NA	2.38	1.41	1.37
6	A	582	SRM	CDA-C2A	2.41	1.60	1.56
6	B	581	SRM	CAA-C3A	2.54	1.55	1.51
6	D	584	SRM	CAB-C3B	3.04	1.56	1.51
6	E	583	SRM	CMB-C2B	3.16	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	582	SRM	CAB-C3B	3.18	1.57	1.51
6	B	581	SRM	CMB-C2B	3.44	1.62	1.54
6	D	584	SRM	CMB-C2B	3.50	1.62	1.54
6	A	582	SRM	CMB-C2B	3.57	1.62	1.54
6	B	581	SRM	CAB-C3B	3.62	1.57	1.51
6	A	582	SRM	FE-NB	3.71	2.10	1.95
6	E	583	SRM	CAB-C3B	3.79	1.58	1.51
6	D	584	SRM	FE-NA	3.84	2.11	1.95
6	D	584	SRM	FE-NB	4.05	2.11	1.95
6	A	582	SRM	FE-NA	4.07	2.11	1.95

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	581	SRM	CAB-C3B-C2B	-15.96	105.49	123.46
6	E	583	SRM	CAB-C3B-C2B	-15.89	105.57	123.46
6	D	584	SRM	CAB-C3B-C2B	-15.71	105.77	123.46
6	A	582	SRM	CAB-C3B-C2B	-15.35	106.18	123.46
6	B	581	SRM	CAA-C3A-C2A	-9.41	112.86	123.46
6	E	583	SRM	CAA-C3A-C2A	-9.23	113.07	123.46
6	E	583	SRM	CBD-CAD-C2D	-4.99	103.59	112.53
6	B	581	SRM	CBD-CAD-C2D	-4.82	103.90	112.53
6	A	582	SRM	CAA-C3A-C2A	-4.74	118.12	123.46
6	D	584	SRM	CAA-C3A-C2A	-4.67	118.21	123.46
6	B	581	SRM	CDD-C3D-C4D	-2.74	122.89	127.34
6	E	583	SRM	CDD-C3D-C4D	-2.67	123.01	127.34
6	E	583	SRM	CDC-C2C-C1C	-2.55	123.26	127.38
6	B	581	SRM	CDC-C2C-C1C	-2.52	123.32	127.38
6	A	582	SRM	CDD-C3D-C4D	-2.44	123.37	127.34
6	D	584	SRM	CDD-C3D-C4D	-2.22	123.74	127.34
6	B	581	SRM	CBC-CAC-C3C	2.02	116.15	112.53
6	E	583	SRM	C4D-C3D-C2D	2.05	109.24	106.70
6	E	583	SRM	CMB-C2B-CDB	2.13	112.29	109.76
6	E	583	SRM	CBC-CAC-C3C	2.22	116.51	112.53
6	B	581	SRM	C3A-C4A-NA	2.24	110.89	107.60
6	A	582	SRM	CBC-CAC-C3C	2.31	116.67	112.53
6	E	583	SRM	C3A-C4A-NA	2.34	111.04	107.60
6	E	583	SRM	C2B-C1B-NB	2.50	112.56	107.99
6	B	581	SRM	C2B-C1B-NB	2.54	112.64	107.99
6	D	584	SRM	CBC-CAC-C3C	2.60	117.19	112.53
6	B	581	SRM	CAD-CBD-CCD	2.65	117.60	112.75
6	E	583	SRM	CAA-CBA-CCA	2.75	117.79	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	583	SRM	CAD-CBD-CCD	2.85	117.97	112.75
6	B	581	SRM	CAA-CBA-CCA	3.03	118.31	112.75
6	B	581	SRM	C4D-CHA-C1A	3.13	132.12	127.83
6	E	583	SRM	C4D-CHA-C1A	3.14	132.14	127.83
6	D	584	SRM	CMA-C2A-CDA	3.22	113.60	109.76
6	D	584	SRM	C4B-NB-C1B	3.73	108.93	106.90
6	A	582	SRM	CMA-C2A-CDA	4.08	114.61	109.76
6	A	582	SRM	C4B-NB-C1B	4.10	109.13	106.90
6	B	581	SRM	C2B-CDB-CEB	4.11	121.81	115.45
6	E	583	SRM	C2B-CDB-CEB	4.47	122.37	115.45
6	A	582	SRM	C4A-NA-C1A	4.64	109.42	106.90
6	D	584	SRM	C4A-NA-C1A	4.89	109.56	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	582	SRM	9	0
5	A	6573	SO3	2	0
4	A	802	SF4	1	0
6	B	581	SRM	6	0
4	B	803	SF4	2	0
6	D	584	SRM	15	0
4	D	806	SF4	1	0
6	E	583	SRM	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	435/435 (100%)	0.01	6 (1%) 78 82	8, 15, 32, 60	0
1	D	435/435 (100%)	-0.15	5 (1%) 82 86	6, 12, 26, 60	0
2	B	385/385 (100%)	0.01	8 (2%) 67 72	8, 15, 28, 46	1 (0%)
2	E	385/385 (100%)	-0.08	4 (1%) 84 87	6, 13, 29, 54	0
3	C	104/104 (100%)	1.29	23 (22%) 1 1	23, 36, 59, 74	1 (0%)
3	F	104/104 (100%)	0.31	5 (4%) 34 40	15, 25, 34, 50	0
All	All	1848/1848 (100%)	0.04	51 (2%) 56 63	6, 15, 35, 74	2 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	HIS	6.8
2	E	244	ASN	6.1
2	B	2	ALA	5.5
3	F	105	VAL	4.8
3	C	8	GLY	4.8
1	D	3	LYS	4.6
3	C	6	PHE	4.6
3	C	105	VAL	4.3
2	B	188[A]	CYS	4.3
3	C	23	ASP	4.1
3	C	104[A]	CYS	4.1
2	E	246	GLN	3.7
3	F	26	CYS	3.7
3	C	40	GLY	3.6
3	C	10	ALA	3.5
3	F	23	ASP	3.4
2	B	120	THR	3.4
1	A	4	HIS	3.4
3	C	3	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	386	SER	3.2
3	C	9	SER	3.1
3	C	4	VAL	3.1
3	C	32	TYR	3.0
3	C	7	ALA	2.8
3	F	8	GLY	2.8
3	F	40	GLY	2.7
2	B	246	GLN	2.7
3	C	26	CYS	2.7
1	A	33	LYS	2.6
1	A	273	LYS	2.6
1	A	418	GLU	2.6
1	D	416	LYS	2.6
3	C	11	PHE	2.5
1	D	430	ASP	2.5
2	E	216	GLU	2.5
3	C	34	LYS	2.5
3	C	51	ASP	2.4
3	C	76	LYS	2.4
3	C	25	TRP	2.4
1	D	425	SER	2.3
2	B	243	VAL	2.3
1	A	89	GLU	2.3
3	C	5	GLU	2.3
2	B	169	LEU	2.3
2	B	3	PHE	2.3
1	A	433	LYS	2.2
2	B	109	GLU	2.2
3	C	12	GLU	2.1
3	C	55	ASP	2.1
3	C	74	GLY	2.1
3	C	44	ALA	2.1

## 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	SO3	D	6575	4/4	0.72	0.29	4.53	67,67,67,68	0
6	SRM	B	581	62/63	0.89	0.20	3.09	11,18,22,33	0
6	SRM	E	583	62/63	0.90	0.17	3.06	8,12,16,30	0
5	SO3	A	6573	4/4	0.44	0.28	2.76	68,68,68,70	0
6	SRM	D	584	63/63	0.93	0.15	0.61	7,14,22,30	0
5	SO3	D	6576	4/4	0.96	0.12	0.55	21,22,25,25	0
6	SRM	A	582	63/63	0.92	0.15	0.24	11,16,24,30	0
4	SF4	D	806	8/8	0.96	0.10	-0.27	9,11,12,13	0
5	SO3	A	6574	4/4	0.96	0.09	-0.77	24,25,26,28	0
4	SF4	A	802	8/8	0.98	0.10	-0.89	13,14,15,15	0
4	SF4	B	803	7/8	0.97	0.08	-0.99	14,14,16,17	0
4	SF4	A	801	8/8	0.95	0.09	-1.07	16,18,19,19	0
4	SF4	D	805	8/8	0.97	0.07	-1.23	12,12,13,14	0
4	SF4	E	808	8/8	0.96	0.09	-1.47	18,19,20,21	0
4	SF4	B	804	8/8	0.98	0.08	-1.53	14,15,16,17	0
4	SF4	E	807	7/8	0.97	0.08	-1.97	14,14,17,18	0

## 6.5 Other polymers

There are no such residues in this entry.