



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3MMC  
Title : Structure of the dissimilatory sulfite reductase from *Archaeoglobus fulgidus*  
Authors : Schiffer, A.; Parey, K.; Warkentin, E.; Diederichs, K.; Huber, H.; Stetter, K.O.; Kroneck, P.M.H.; Ermler, U.  
Deposited on : 2010-04-19  
Resolution : 2.04 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

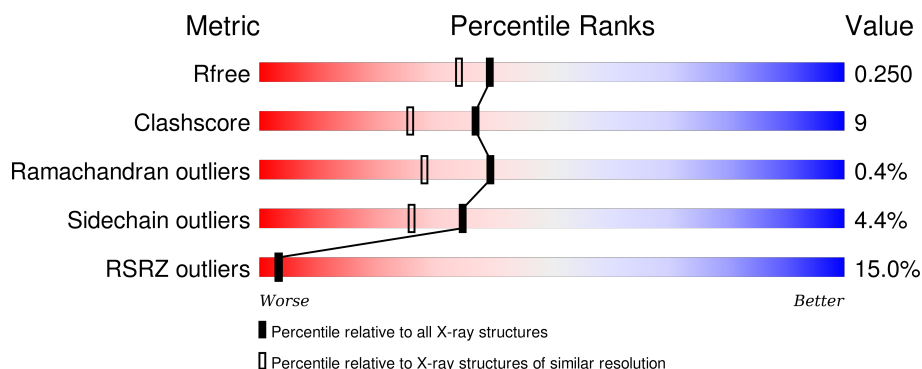
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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	418	<div> <div>3%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	D	418	<div> <div>28%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
2	B	366	<div> <div>%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
2	E	366	<div> <div>28%</div> <div>76%</div> <div>21%</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
3	SRM	D	580	-	-	-	X
3	SRM	E	570	-	-	-	X
4	SF4	D	575	-	-	X	X
4	SF4	E	585	-	-	X	X
5	GOL	A	590	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13324 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.

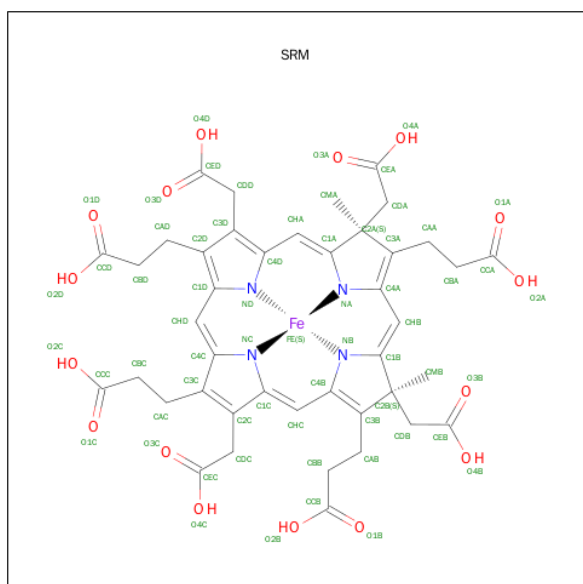
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3329	2134	557	612	26			
1	D	417	Total	C	N	O	S	0	0	0
			3329	2134	557	612	26			

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

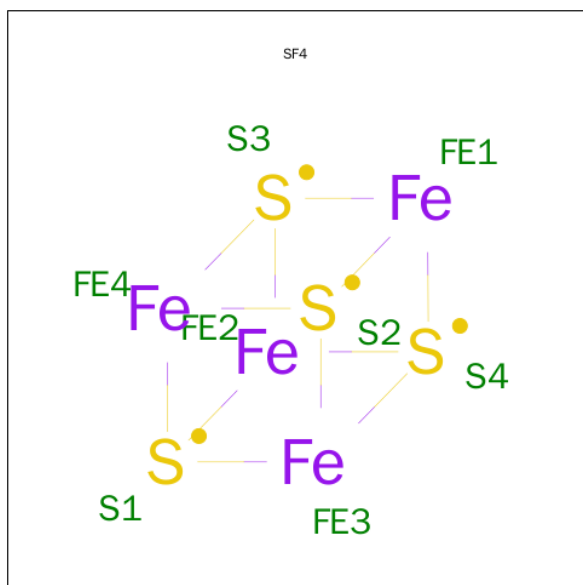
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			
2	E	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			

- 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: Fe<sub>4</sub>S<sub>4</sub>).



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 GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

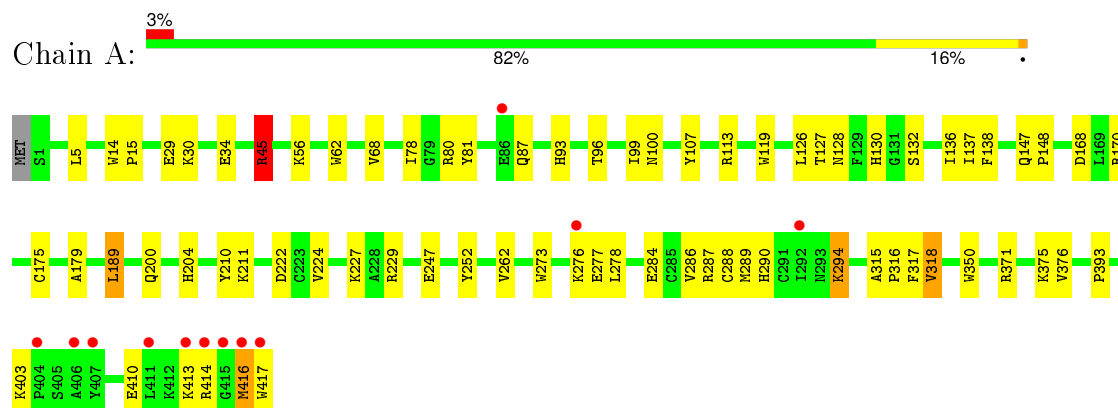
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	220	Total	O	0	0
			220	220		
6	B	265	Total	O	0	0
			265	265		
6	D	39	Total	O	0	0
			39	39		
6	E	18	Total	O	0	0
			18	18		

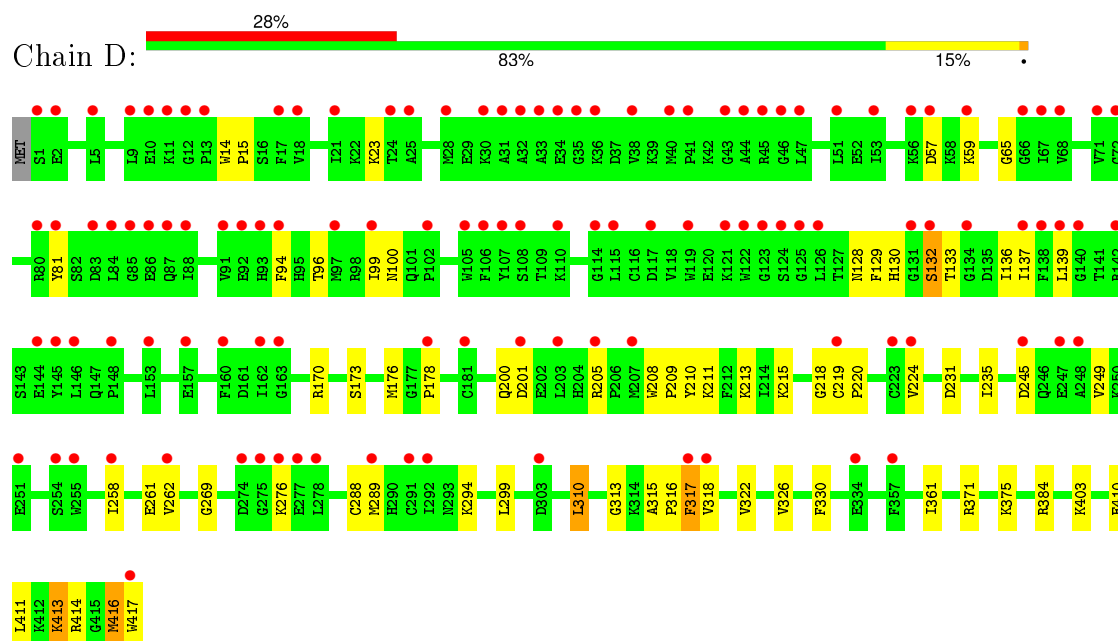
### 3 Residue-property plots

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.

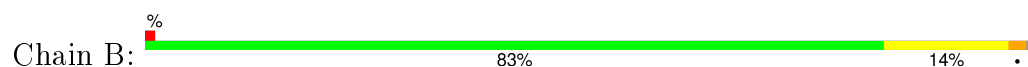
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

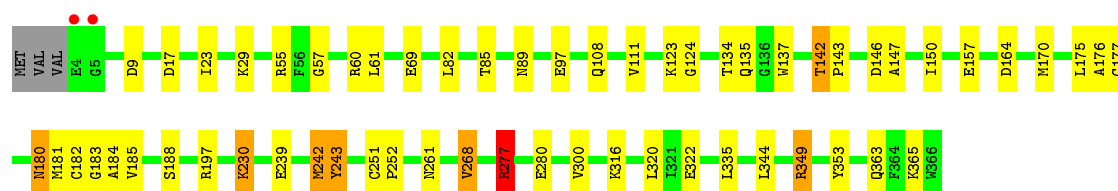


- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

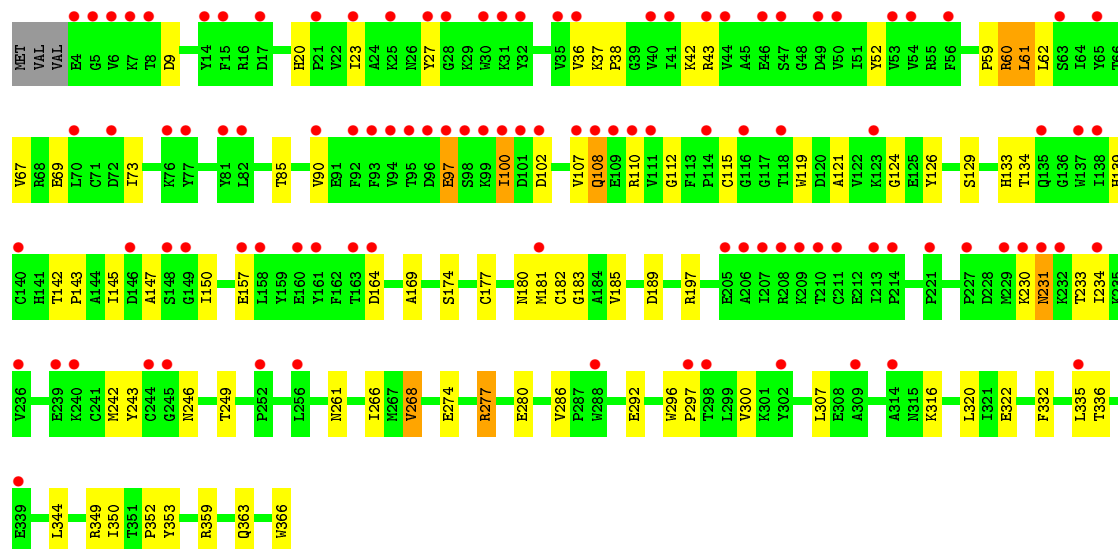
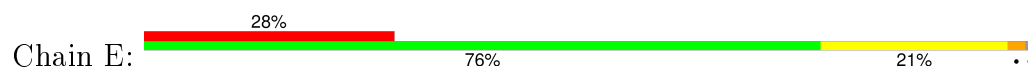


- Molecule 2: Sulfite reductase, dissimilatory-type subunit beta





- 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, $\alpha$ , $\beta$ , $\gamma$	94.91Å 69.26Å 147.21Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	20.11 – 2.04 20.07 – 2.04	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.11-2.04) 97.9 (20.07-2.04)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, $R_{free}$	0.186 , 0.223 0.223 , 0.250	Depositor DCC
$R_{free}$ test set	5736 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.5	EDS
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 114053 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13324	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.80	1/3416 (0.0%)	0.78	4/4610 (0.1%)
1	D	0.51	1/3416 (0.0%)	0.60	0/4610
2	B	0.85	0/2984	0.83	6/4058 (0.1%)
2	E	0.52	1/2984 (0.0%)	0.65	0/4058
All	All	0.69	3/12800 (0.0%)	0.72	10/17336 (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	1
2	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	23	LYS	CD-CE	7.93	1.71	1.51
2	E	115	CYS	CB-SG	6.95	1.94	1.82
1	A	175	CYS	CB-SG	-5.71	1.72	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	277	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	45	ARG	NE-CZ-NH2	-6.41	117.09	120.30
2	B	277	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	189	LEU	CB-CG-CD1	6.07	121.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	B	55	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	318	VAL	N-CA-C	5.86	126.83	111.00
1	A	287	ARG	NE-CZ-NH2	-5.37	117.62	120.30
2	B	164	ASP	CB-CG-OD2	5.33	123.10	118.30
2	B	17	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	PHE	Peptide
2	B	180	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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	3329	0	3276	57	0
1	D	3329	0	3276	57	0
2	B	2901	0	2838	62	0
2	E	2901	0	2838	78	0
3	A	63	0	34	7	0
3	B	63	0	34	2	0
3	D	63	0	34	16	0
3	E	63	0	34	13	0
4	A	16	0	0	0	0
4	B	16	0	0	1	0
4	D	16	0	0	2	0
4	E	16	0	0	3	0
5	A	6	0	8	8	0
6	A	220	0	0	2	0
6	B	265	0	0	16	0
6	D	39	0	0	5	0
6	E	18	0	0	2	0
All	All	13324	0	12372	236	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 9.

All (236) 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:134:THR:HG21	2:E:182:CYS:HB2	1.39	1.00
3:D:580:SRM:HMB3	2:E:182:CYS:HA	1.50	0.93
2:E:177:CYS:HB2	4:E:585:SF4:S3	2.09	0.92
2:B:134:THR:CG2	6:B:4370:HOH:O	2.17	0.92
2:B:69:GLU:HG2	6:B:4358:HOH:O	1.70	0.92
2:E:90:VAL:HG23	6:E:4492:HOH:O	1.70	0.90
3:E:570:SRM:HBD1	3:E:570:SRM:HDD1	1.51	0.89
1:A:403:LYS:H	2:E:261:ASN:HD21	1.20	0.89
4:D:575:SF4:S4	6:E:4464:HOH:O	2.32	0.86
2:E:134:THR:CG2	2:E:182:CYS:HB2	2.05	0.85
1:D:128:ASN:HB2	1:D:137:ILE:HB	1.58	0.85
2:B:124:GLY:HA3	2:B:316:LYS:HD2	1.60	0.83
1:A:170:ARG:HH22	5:A:590:GOL:H11	1.42	0.83
2:B:183:GLY:N	6:B:4408:HOH:O	2.14	0.81
2:B:60:ARG:HB2	6:B:4420:HOH:O	1.81	0.80
2:E:134:THR:HB	4:E:585:SF4:S4	2.22	0.79
2:E:124:GLY:HA3	2:E:316:LYS:HD2	1.65	0.79
2:B:185:VAL:CG2	6:B:4392:HOH:O	2.30	0.79
2:B:134:THR:HG21	6:B:4370:HOH:O	1.82	0.79
1:D:316:PRO:HG2	2:E:181:MET:HE3	1.67	0.77
3:D:580:SRM:HAB2	2:E:183:GLY:H	1.46	0.76
2:B:182:CYS:C	6:B:4408:HOH:O	2.24	0.76
2:E:52:TYR:CE1	2:E:97:GLU:HB3	2.20	0.76
1:A:211:LYS:HZ3	5:A:590:GOL:H32	1.51	0.75
2:B:261:ASN:HD21	1:D:403:LYS:H	1.32	0.75
1:A:211:LYS:NZ	5:A:590:GOL:H32	2.02	0.73
1:D:316:PRO:HG2	2:E:181:MET:CE	2.19	0.72
2:E:230:LYS:CB	2:E:231:ASN:HB2	2.19	0.72
1:A:371:ARG:O	1:A:375:LYS:HD3	1.90	0.72
3:A:580:SRM:HHB	3:A:580:SRM:HBA1	1.71	0.71
1:A:128:ASN:HD21	2:B:135:GLN:HE22	1.36	0.70
1:A:128:ASN:ND2	2:B:135:GLN:HE22	1.89	0.70
1:A:316:PRO:HG2	2:B:181:MET:HE3	1.72	0.70
1:A:286:VAL:HG23	2:B:363:GLN:HG2	1.74	0.69
2:E:42:LYS:HG3	2:E:52:TYR:CE2	2.28	0.69
1:D:211:LYS:HZ3	3:D:580:SRM:HDA2	1.59	0.67
1:D:176:MET:CE	3:E:570:SRM:HBA2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:ASP:C	6:B:4376:HOH:O	2.32	0.66
1:D:132:SER:HB2	3:D:580:SRM:HBB2	1.76	0.66
1:A:211:LYS:HZ3	5:A:590:GOL:C3	2.08	0.66
2:E:85:THR:HB	3:E:570:SRM:HAB2	1.77	0.66
1:D:14:TRP:CD2	1:D:15:PRO:HD2	2.31	0.65
2:E:230:LYS:HB2	2:E:231:ASN:ND2	2.12	0.64
2:E:119:TRP:HE1	3:E:570:SRM:HDD2	1.63	0.64
2:B:185:VAL:HG21	6:B:4392:HOH:O	1.95	0.64
1:D:211:LYS:NZ	3:D:580:SRM:HDA2	2.12	0.63
2:E:197:ARG:HH21	2:E:261:ASN:HD22	1.43	0.63
1:A:316:PRO:HG2	2:B:181:MET:CE	2.27	0.63
1:D:288:CYS:O	1:D:289:MET:HB2	1.97	0.62
1:A:14:TRP:CD2	1:A:15:PRO:HD2	2.35	0.62
2:E:157:GLU:HG3	2:E:300:VAL:HG11	1.82	0.62
2:E:230:LYS:CA	2:E:231:ASN:HB2	2.29	0.62
1:A:107:TYR:OH	1:A:130:HIS:HE1	1.83	0.61
1:A:262:VAL:HG22	1:A:294:LYS:HG2	1.82	0.61
1:D:261:GLU:HB3	1:D:294:LYS:HE2	1.81	0.61
2:E:266:ILE:HB	2:E:286:VAL:HB	1.84	0.60
1:A:375:LYS:HD2	1:A:375:LYS:N	2.17	0.59
1:A:229:ARG:CD	2:B:184:ALA:HB2	2.32	0.59
1:A:170:ARG:HH12	5:A:590:GOL:H31	1.68	0.58
2:E:292:GLU:HB2	2:E:296:TRP:HA	1.85	0.58
1:A:170:ARG:HH12	5:A:590:GOL:C3	2.16	0.58
2:E:230:LYS:HB2	2:E:231:ASN:HB2	1.86	0.57
1:A:315:ALA:HB1	1:A:316:PRO:HD2	1.87	0.57
2:B:85:THR:HB	3:B:570:SRM:HAB1	1.87	0.56
2:B:147:ALA:HB2	2:B:177:CYS:SG	2.45	0.56
2:B:177:CYS:HB2	4:B:585:SF4:S3	2.46	0.56
2:B:261:ASN:HD21	1:D:403:LYS:N	2.04	0.56
1:D:200:GLN:HE21	2:E:9:ASP:HA	1.70	0.56
3:A:580:SRM:CBB	3:A:580:SRM:CMB	2.84	0.56
2:E:43:ARG:NH2	3:E:570:SRM:O4A	2.32	0.55
1:D:213:LYS:HZ1	3:D:580:SRM:HDB2	1.70	0.55
3:E:570:SRM:CBA	3:E:570:SRM:HHB	2.36	0.55
1:A:119:TRP:CH2	1:A:138:PHE:HB3	2.42	0.55
1:A:276:LYS:HG2	1:A:277:GLU:HG2	1.89	0.55
1:D:258:ILE:HA	1:D:262:VAL:HG23	1.89	0.55
2:B:175:LEU:C	2:B:175:LEU:HD23	2.28	0.54
1:D:57:ASP:HB3	1:D:59:LYS:HG2	1.89	0.54
1:A:286:VAL:CG2	2:B:363:GLN:HG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:SER:HB2	3:D:580:SRM:CBB	2.38	0.53
1:D:213:LYS:NZ	3:D:580:SRM:HDB2	2.23	0.53
3:E:570:SRM:O4D	3:E:570:SRM:HHA	2.08	0.53
2:E:20:HIS:HB3	2:E:23:ILE:HD12	1.90	0.53
1:D:14:TRP:CG	1:D:15:PRO:HD2	2.44	0.53
2:E:230:LYS:HB2	2:E:231:ASN:CB	2.39	0.53
1:A:29:GLU:OE2	1:A:45:ARG:HD2	2.09	0.53
1:A:127:THR:O	2:B:61:LEU:HD12	2.08	0.53
2:B:57:GLY:HA2	2:B:89:ASN:ND2	2.23	0.53
1:D:262:VAL:HG22	1:D:294:LYS:HG2	1.90	0.53
1:A:30:LYS:O	1:A:34:GLU:HG3	2.09	0.52
2:B:134:THR:HG21	2:B:182:CYS:HB2	1.92	0.52
2:B:146:ASP:O	2:B:150:ILE:HD12	2.10	0.52
1:A:229:ARG:HD3	2:B:184:ALA:HB2	1.92	0.51
2:B:268:VAL:HG13	2:B:320:LEU:CD2	2.40	0.51
1:D:416:MET:O	1:D:417:TRP:HB3	2.09	0.51
1:D:178:PRO:HG2	2:E:27:TYR:CZ	2.46	0.51
2:B:277:ARG:NH2	2:B:280:GLU:OE1	2.40	0.51
1:D:245:ASP:O	1:D:249:VAL:HG23	2.11	0.51
3:A:580:SRM:HMB3	3:A:580:SRM:HBB2	1.91	0.51
2:B:184:ALA:HB3	6:B:4380:HOH:O	2.10	0.50
2:B:349:ARG:NH2	2:E:350:ILE:O	2.44	0.50
1:D:170:ARG:HG3	1:D:213:LYS:HE2	1.94	0.50
1:D:235:ILE:HD12	1:D:310:LEU:HD22	1.93	0.50
2:B:137:TRP:CE3	2:B:146:ASP:HB2	2.46	0.50
1:D:261:GLU:HB3	1:D:294:LYS:CE	2.42	0.50
1:A:416:MET:O	1:A:417:TRP:HB3	2.12	0.50
1:D:99:ILE:HB	1:D:136:ILE:HB	1.92	0.50
1:D:261:GLU:CD	2:E:316:LYS:HE3	2.32	0.49
1:D:317:PHE:CD2	2:E:180:ASN:ND2	2.80	0.49
2:E:134:THR:CG2	2:E:182:CYS:CB	2.84	0.49
1:A:403:LYS:N	2:E:261:ASN:HD21	1.98	0.49
1:A:262:VAL:HG22	1:A:294:LYS:CG	2.42	0.49
2:E:121:ALA:CB	3:E:570:SRM:O3D	2.61	0.49
2:E:69:GLU:HG2	2:E:110:ARG:HH21	1.78	0.49
2:E:268:VAL:HG22	2:E:320:LEU:HD22	1.95	0.49
3:A:580:SRM:C2D	2:B:180:ASN:HB2	2.43	0.49
1:A:62:TRP:HB3	1:A:80:ARG:HD2	1.95	0.49
2:E:230:LYS:HB2	2:E:231:ASN:HD22	1.79	0.48
1:A:410:GLU:O	1:A:414:ARG:HG2	2.13	0.48
2:E:37:LYS:HB2	2:E:38:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:580:SRM:CAB	2:E:183:GLY:H	2.22	0.48
1:A:416:MET:O	1:A:417:TRP:CB	2.61	0.48
2:E:277:ARG:HG2	2:E:322:GLU:HG2	1.95	0.48
1:A:99:ILE:HB	1:A:136:ILE:HB	1.94	0.48
2:B:157:GLU:HG3	2:B:300:VAL:HG11	1.95	0.48
2:B:175:LEU:HD23	2:B:176:ALA:N	2.30	0.47
3:E:570:SRM:HDD1	3:E:570:SRM:CBD	2.26	0.47
2:B:134:THR:HG23	6:B:4370:HOH:O	1.97	0.47
1:D:315:ALA:HB1	1:D:316:PRO:CD	2.45	0.47
3:E:570:SRM:HBA1	3:E:570:SRM:HHB	1.95	0.47
2:B:197:ARG:HH21	2:B:261:ASN:HD22	1.63	0.47
2:E:145:ILE:HD12	2:E:150:ILE:HD12	1.96	0.47
2:E:142:THR:N	2:E:143:PRO:HD3	2.29	0.47
1:D:218:GLY:HA3	4:D:575:SF4:S2	2.54	0.46
1:D:173:SER:OG	1:D:215:LYS:HG2	2.15	0.46
1:D:416:MET:O	1:D:417:TRP:CB	2.63	0.46
1:D:213:LYS:NZ	3:D:580:SRM:CDB	2.78	0.46
2:E:296:TRP:N	2:E:297:PRO:HD3	2.30	0.46
3:D:580:SRM:HDD1	3:D:580:SRM:CCD	2.46	0.46
2:B:60:ARG:HD3	6:B:4420:HOH:O	2.15	0.46
1:D:129:PHE:HA	1:D:130:HIS:HA	1.73	0.46
2:E:197:ARG:NH2	2:E:261:ASN:HD22	2.12	0.46
2:E:189:ASP:O	2:E:268:VAL:HA	2.16	0.46
1:D:213:LYS:HZ2	3:D:580:SRM:HDB1	1.81	0.45
1:D:411:LEU:HD13	1:D:417:TRP:HA	1.98	0.45
2:E:147:ALA:HB2	2:E:177:CYS:SG	2.56	0.45
2:E:108:GLN:H	2:E:108:GLN:HE21	1.64	0.45
1:A:130:HIS:HD2	6:B:4031:HOH:O	1.99	0.45
1:A:290:HIS:O	1:A:294:LYS:HB2	2.15	0.45
1:D:317:PHE:HD2	2:E:180:ASN:HD22	1.65	0.45
2:E:73:ILE:HD13	2:E:107:VAL:HG22	1.99	0.45
1:D:176:MET:HE1	3:E:570:SRM:HBA2	1.95	0.45
1:A:119:TRP:CZ3	1:A:138:PHE:HB3	2.52	0.45
2:B:251:CYS:HA	2:B:252:PRO:HD2	1.84	0.45
3:E:570:SRM:HAC2	3:E:570:SRM:HCD1	1.78	0.45
2:B:349:ARG:HH22	2:E:352:PRO:HD3	1.82	0.45
2:E:142:THR:N	2:E:143:PRO:CD	2.79	0.45
1:A:284:GLU:HA	2:B:365:LYS:HD3	1.99	0.45
3:D:580:SRM:HAA1	3:D:580:SRM:HDA1	1.71	0.45
2:B:29:LYS:HE3	6:B:4374:HOH:O	2.17	0.45
2:B:182:CYS:CB	6:B:4408:HOH:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:CYS:O	1:A:289:MET:HB2	2.16	0.45
1:A:211:LYS:NZ	5:A:590:GOL:C3	2.71	0.44
1:A:81:TYR:CE2	1:A:93:HIS:CD2	3.05	0.44
1:D:201:ASP:OD1	1:D:205:ARG:HD2	2.18	0.44
2:E:126:TYR:CE1	2:E:169:ALA:HA	2.52	0.44
1:A:222:ASP:OD1	1:A:227:LYS:NZ	2.48	0.44
2:E:177:CYS:CB	4:E:585:SF4:S3	2.95	0.44
2:B:268:VAL:HG13	2:B:320:LEU:HD22	1.99	0.44
1:A:393:PRO:HG3	2:E:181:MET:HE2	2.00	0.44
6:D:4535:HOH:O	2:E:182:CYS:SG	2.62	0.44
2:B:142:THR:N	2:B:143:PRO:CD	2.81	0.44
1:A:128:ASN:HB2	1:A:137:ILE:HB	2.00	0.43
2:B:277:ARG:HG2	2:B:322:GLU:HG2	1.99	0.43
1:D:208:TRP:HB3	1:D:209:PRO:CD	2.48	0.43
1:D:219:CYS:HB2	1:D:220:PRO:CD	2.48	0.43
1:D:330:PHE:HB2	2:E:366:TRP:CH2	2.53	0.43
1:D:176:MET:HE2	3:E:570:SRM:HBA2	1.99	0.43
1:D:139:LEU:HD11	2:E:139:HIS:CG	2.54	0.43
1:D:65:GLY:HA3	1:D:81:TYR:CD1	2.53	0.43
2:E:119:TRP:HB2	2:E:126:TYR:CD2	2.53	0.43
2:B:349:ARG:NH2	2:E:352:PRO:HD3	2.34	0.43
1:D:129:PHE:HB2	2:E:62:LEU:HD22	1.99	0.43
1:A:168:ASP:OD1	1:A:170:ARG:HD3	2.19	0.43
2:B:176:ALA:HB1	2:B:181:MET:HA	2.00	0.43
2:B:268:VAL:HG13	2:B:320:LEU:HD21	2.01	0.43
1:A:273:TRP:HB2	1:A:278:LEU:HD12	2.01	0.43
2:E:62:LEU:HD23	2:E:67:VAL:HG22	2.01	0.43
1:D:410:GLU:O	1:D:414:ARG:HG2	2.18	0.43
2:B:82:LEU:HD23	2:B:82:LEU:N	2.34	0.42
1:A:229:ARG:HD2	2:B:184:ALA:N	2.33	0.42
1:A:96:THR:HG21	6:A:4356:HOH:O	2.19	0.42
1:D:310:LEU:HD12	1:D:326:VAL:HA	2.00	0.42
2:E:174:SER:HB3	2:E:185:VAL:HG22	2.02	0.42
1:A:179:ALA:O	2:B:23:ILE:HG23	2.19	0.42
2:E:332:PHE:CE1	2:E:336:THR:HG21	2.55	0.42
1:D:384:ARG:O	2:E:359:ARG:HD2	2.19	0.42
3:A:580:SRM:CMB	3:A:580:SRM:HBB2	2.49	0.42
2:E:277:ARG:NH2	2:E:280:GLU:OE1	2.52	0.42
2:E:60:ARG:HD3	2:E:133:HIS:CE1	2.55	0.42
1:D:315:ALA:HB3	3:D:580:SRM:HBA1	2.02	0.42
1:D:128:ASN:OD1	2:E:60:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:42:LYS:HE2	2:E:42:LYS:HB3	1.86	0.42
1:D:403:LYS:NZ	6:D:4208:HOH:O	2.52	0.42
3:A:580:SRM:O3B	2:B:135:GLN:HG2	2.18	0.42
2:E:59:PRO:O	2:E:61:LEU:N	2.53	0.42
1:D:269:GLY:HA2	6:D:4331:HOH:O	2.19	0.42
3:D:580:SRM:HMB1	3:D:580:SRM:HAB1	1.85	0.42
2:E:108:GLN:N	2:E:108:GLN:HE21	2.18	0.42
1:A:81:TYR:HE2	1:A:93:HIS:CD2	2.38	0.42
1:D:231:ASP:HB3	1:D:361:ILE:CG2	2.50	0.42
1:A:170:ARG:NH1	5:A:590:GOL:H31	2.34	0.41
1:A:147:GLN:HB3	1:A:148:PRO:CD	2.50	0.41
2:B:353:TYR:HA	2:E:353:TYR:HA	2.02	0.41
2:E:246:ASN:O	2:E:249:THR:HB	2.20	0.41
3:A:580:SRM:HHB	3:A:580:SRM:CBA	2.47	0.41
2:B:242:MET:C	2:B:243:TYR:CG	2.93	0.41
2:B:182:CYS:HB3	6:B:4408:HOH:O	2.21	0.41
2:E:230:LYS:N	2:E:231:ASN:HB2	2.36	0.41
1:A:375:LYS:N	1:A:375:LYS:CD	2.81	0.41
2:B:170:MET:SD	3:B:570:SRM:HBD1	2.60	0.41
3:D:580:SRM:CHD	6:D:4535:HOH:O	2.69	0.41
1:A:200:GLN:HE21	2:B:9:ASP:HA	1.85	0.41
2:B:69:GLU:OE2	2:B:111:VAL:HG12	2.20	0.41
2:E:230:LYS:HB2	2:E:231:ASN:CG	2.41	0.41
1:A:200:GLN:NE2	1:A:204:HIS:NE2	2.69	0.41
1:D:413:LYS:HE2	6:D:4364:HOH:O	2.21	0.41
1:A:252:TYR:OH	6:A:4162:HOH:O	2.17	0.41
2:E:100:ILE:H	2:E:100:ILE:HG13	1.61	0.41
1:A:350:TRP:CG	1:A:376:VAL:HG21	2.55	0.41
2:B:185:VAL:HG23	2:B:185:VAL:H	1.50	0.40
2:E:108:GLN:HA	2:E:112:GLY:HA2	2.02	0.40
2:B:230:LYS:H	2:B:230:LYS:HG2	1.59	0.40
1:A:113:ARG:HH11	1:A:113:ARG:HD2	1.77	0.40
2:E:274:GLU:OE1	2:E:363:GLN:HG3	2.21	0.40
1:D:313:GLY:HA2	1:D:322:VAL:O	2.21	0.40
2:E:233:THR:OG1	2:E:234:ILE:N	2.54	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%)	402 (97%)	12 (3%)	1 (0%)	52	43
1	D	415/418 (99%)	395 (95%)	19 (5%)	1 (0%)	52	43
2	B	361/366 (99%)	346 (96%)	14 (4%)	1 (0%)	46	36
2	E	361/366 (99%)	324 (90%)	34 (9%)	3 (1%)	24	12
All	All	1552/1568 (99%)	1467 (94%)	79 (5%)	6 (0%)	39	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	VAL
2	E	231	ASN
2	E	60	ARG
1	D	318	VAL
2	E	36	VAL
2	B	142	THR

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/354 (100%)	337 (96%)	16 (4%)	34	25
1	D	353/354 (100%)	338 (96%)	15 (4%)	36	28
2	B	314/317 (99%)	301 (96%)	13 (4%)	37	28
2	E	314/317 (99%)	299 (95%)	15 (5%)	31	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1334/1342 (99%)	1275 (96%)	59 (4%)	35 26

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	45	ARG
1	A	56	LYS
1	A	68	VAL
1	A	78	ILE
1	A	87	GLN
1	A	100	ASN
1	A	126	LEU
1	A	132	SER
1	A	189	LEU
1	A	210	TYR
1	A	224	VAL
1	A	247	GLU
1	A	294	LYS
1	A	413	LYS
1	A	416	MET
2	B	97	GLU
2	B	108	GLN
2	B	123	LYS
2	B	188	SER
2	B	230	LYS
2	B	239	GLU
2	B	242	MET
2	B	243	TYR
2	B	268	VAL
2	B	277	ARG
2	B	335	LEU
2	B	344	LEU
2	B	349	ARG
1	D	94	PHE
1	D	96	THR
1	D	100	ASN
1	D	132	SER
1	D	133	THR
1	D	210	TYR
1	D	224	VAL
1	D	276	LYS

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Mol	Chain	Res	Type
1	D	299	LEU
1	D	310	LEU
1	D	317	PHE
1	D	371	ARG
1	D	375	LYS
1	D	413	LYS
1	D	416	MET
2	E	61	LEU
2	E	97	GLU
2	E	100	ILE
2	E	102	ASP
2	E	108	GLN
2	E	129	SER
2	E	164	ASP
2	E	242	MET
2	E	243	TYR
2	E	268	VAL
2	E	277	ARG
2	E	307	LEU
2	E	335	LEU
2	E	344	LEU
2	E	349	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	128	ASN
1	A	130	HIS
1	A	200	GLN
2	B	89	ASN
2	B	180	ASN
2	B	261	ASN
2	B	313	ASN
2	B	363	GLN
1	D	100	ASN
1	D	200	GLN
2	E	89	ASN
2	E	180	ASN
2	E	231	ASN
2	E	261	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	2.02	6 (20%)	29,112,112	4.10	10 (34%)
5	GOL	A	590	-	5,5,5	0.47	0	5,5,5	0.98	0
3	SRM	B	570	1	29,70,70	2.11	8 (27%)	29,112,112	4.96	18 (62%)
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	0,12,12	0.00	-	0,24,24	0.00	-
3	SRM	D	580	-	29,70,70	2.12	9 (31%)	29,112,112	4.54	15 (51%)
3	SRM	E	570	1	29,70,70	2.66	10 (34%)	29,112,112	4.98	15 (51%)
4	SF4	E	585	2,6	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	GOL	A	590	-	-	0/4/4/4	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	-	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	-	0/22/126/126	0/0/8/8
4	SF4	E	585	2,6	-	0/0/48/48	0/6/5/5
4	SF4	E	586	2	-	0/0/48/48	0/6/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	570	SRM	C1C-NC	-5.51	1.29	1.36
3	B	570	SRM	C4A-NA	-5.15	1.29	1.39
3	E	570	SRM	C4C-NC	-5.13	1.29	1.36
3	E	570	SRM	C1B-NB	-4.50	1.31	1.38
3	E	570	SRM	C4A-NA	-4.30	1.31	1.39
3	A	580	SRM	C4A-NA	-3.55	1.32	1.39
3	B	570	SRM	C1B-NB	-3.46	1.32	1.38
3	B	570	SRM	C4C-NC	-3.31	1.32	1.36
3	E	570	SRM	C1A-NA	-3.18	1.33	1.38
3	D	580	SRM	C1A-NA	-2.50	1.34	1.38
3	D	580	SRM	C4A-NA	-2.47	1.34	1.39
3	D	580	SRM	C1C-NC	-2.46	1.33	1.36
3	D	580	SRM	C4C-NC	-2.39	1.33	1.36
3	E	570	SRM	C4B-NB	-2.36	1.34	1.39
3	A	580	SRM	C4C-NC	-2.29	1.33	1.36
3	D	580	SRM	C4B-NB	-2.24	1.34	1.39
3	E	570	SRM	CHB-C4A	-2.07	1.34	1.39
3	B	570	SRM	C1C-NC	-2.06	1.33	1.36
3	B	570	SRM	CAB-C3B	2.25	1.55	1.51
3	B	570	SRM	CAA-C3A	2.28	1.55	1.51
3	E	570	SRM	CAA-C3A	2.62	1.56	1.51
3	D	580	SRM	FE-NB	2.99	2.07	1.95
3	A	580	SRM	FE-NB	3.13	2.08	1.95
3	D	580	SRM	FE-NA	3.37	2.09	1.95
3	A	580	SRM	FE-NA	3.84	2.11	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	580	SRM	C3C-C2C	3.96	1.49	1.37
3	B	570	SRM	C3C-C2C	3.99	1.49	1.37
3	D	580	SRM	C3C-C2C	4.24	1.50	1.37
3	E	570	SRM	C3C-C2C	4.96	1.52	1.37
3	B	570	SRM	C3D-C2D	5.94	1.52	1.39
3	A	580	SRM	C3D-C2D	6.42	1.53	1.39
3	E	570	SRM	C3D-C2D	6.50	1.54	1.39
3	D	580	SRM	C3D-C2D	6.78	1.54	1.39

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	580	SRM	CAB-C3B-C2B	-16.83	104.51	123.46
3	B	570	SRM	CAA-C3A-C2A	-15.36	106.17	123.46
3	D	580	SRM	CAB-C3B-C2B	-11.62	110.38	123.46
3	D	580	SRM	CAD-C2D-C1D	-11.20	114.84	127.01
3	E	570	SRM	CAD-C2D-C1D	-10.32	115.80	127.01
3	E	570	SRM	CDD-C3D-C4D	-10.23	110.71	127.34
3	B	570	SRM	CAB-C3B-C2B	-9.79	112.44	123.46
3	E	570	SRM	CAA-C3A-C2A	-8.83	113.51	123.46
3	B	570	SRM	CBC-CAC-C3C	-8.72	96.90	112.53
3	E	570	SRM	CAC-C3C-C4C	-8.37	117.92	127.01
3	B	570	SRM	C4A-NA-C1A	-8.20	102.45	106.90
3	D	580	SRM	CAA-C3A-C2A	-7.82	114.66	123.46
3	D	580	SRM	CDD-C3D-C4D	-7.78	114.70	127.34
3	E	570	SRM	CDC-C2C-C1C	-7.68	114.98	127.38
3	E	570	SRM	C4A-NA-C1A	-7.68	102.73	106.90
3	B	570	SRM	C3B-C4B-NB	-6.12	103.28	110.09
3	E	570	SRM	CAD-C2D-C3D	-5.80	114.94	129.38
3	A	580	SRM	CMB-C2B-CDB	-5.29	103.46	109.76
3	D	580	SRM	CAD-C2D-C3D	-5.15	116.56	129.38
3	E	570	SRM	CAC-C3C-C2C	-4.84	117.33	129.38
3	B	570	SRM	CEC-CDC-C2C	-4.33	108.03	116.31
3	A	580	SRM	CAC-CBC-CCC	-4.15	105.13	112.75
3	A	580	SRM	CAA-C3A-C2A	-4.04	118.92	123.46
3	E	570	SRM	CHB-C4A-C3A	-3.75	116.96	125.48
3	E	570	SRM	CBC-CAC-C3C	-3.73	105.84	112.53
3	B	570	SRM	CAD-CBD-CCD	-3.68	106.00	112.75
3	D	580	SRM	CEC-CDC-C2C	-3.52	109.58	116.31
3	D	580	SRM	C3A-C4A-NA	-3.51	106.18	110.09
3	A	580	SRM	CAD-C2D-C3D	-3.43	120.86	129.38
3	B	570	SRM	CMA-C2A-CDA	-3.25	105.90	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	580	SRM	CED-CDD-C3D	-3.25	110.10	116.31
3	E	570	SRM	CEC-CDC-C2C	-3.00	110.57	116.31
3	A	580	SRM	CAD-CBD-CCD	-2.91	107.40	112.75
3	D	580	SRM	CAA-CBA-CCA	-2.33	108.48	112.75
3	B	570	SRM	CHB-C4A-C3A	-2.25	120.36	125.48
3	B	570	SRM	CAC-C3C-C2C	-2.07	124.24	129.38
3	B	570	SRM	C2B-CDB-CEB	2.01	118.56	115.45
3	A	580	SRM	C4A-NA-C1A	2.02	108.00	106.90
3	D	580	SRM	C2B-CDB-CEB	2.07	118.66	115.45
3	B	570	SRM	CMB-C2B-CDB	2.08	112.23	109.76
3	B	570	SRM	CED-CDD-C3D	2.14	120.41	116.31
3	E	570	SRM	C2B-CDB-CEB	2.42	119.20	115.45
3	D	580	SRM	CBD-CAD-C2D	2.60	117.19	112.53
3	B	570	SRM	CAC-C3C-C4C	2.85	130.10	127.01
3	D	580	SRM	CMB-C2B-CDB	3.02	113.35	109.76
3	D	580	SRM	CMA-C2A-CDA	3.03	113.36	109.76
3	B	570	SRM	CHC-C4B-NB	3.05	129.64	123.70
3	D	580	SRM	C4B-NB-C1B	3.19	108.63	106.90
3	A	580	SRM	CAC-C3C-C4C	3.30	130.59	127.01
3	E	570	SRM	C2A-CDA-CEA	3.96	121.58	115.45
3	B	570	SRM	CAA-CBA-CCA	4.14	120.33	112.75
3	E	570	SRM	CAA-CBA-CCA	4.65	121.27	112.75
3	A	580	SRM	C2A-CDA-CEA	5.75	124.36	115.45
3	B	570	SRM	C3A-C4A-NA	5.82	116.56	110.09
3	A	580	SRM	CBD-CAD-C2D	6.85	124.81	112.53
3	B	570	SRM	CBD-CAD-C2D	7.25	125.53	112.53
3	E	570	SRM	C3A-C4A-NA	9.24	120.36	110.09
3	D	580	SRM	C4A-NA-C1A	9.78	112.21	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	580	SRM	7	0
5	A	590	GOL	8	0
3	B	570	SRM	2	0
4	B	585	SF4	1	0
4	D	575	SF4	2	0
3	D	580	SRM	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	570	SRM	13	0
4	E	585	SF4	3	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	417/418 (99%)	0.08	12 (2%) 55 62	5, 12, 25, 58	0
1	D	417/418 (99%)	1.37	117 (28%) 1 0	4, 13, 25, 41	0
2	B	363/366 (99%)	-0.06	2 (0%) 90 92	5, 11, 19, 57	0
2	E	363/366 (99%)	1.42	103 (28%) 1 0	2, 12, 33, 54	0
All	All	1560/1568 (99%)	0.70	234 (15%) 3 3	2, 12, 26, 58	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	GLY	7.6
1	D	132	SER	7.3
1	D	67	ILE	7.2
1	D	71	VAL	6.9
2	E	5	GLY	6.6
2	E	4	GLU	6.6
2	E	6	VAL	6.3
2	E	7	LYS	6.0
1	D	86	GLU	6.0
2	E	100	ILE	5.9
1	D	33	ALA	5.8
1	D	51	LEU	5.7
1	D	157	GLU	5.5
1	D	47	LEU	5.3
1	A	413	LYS	5.3
1	D	255	TRP	5.3
1	D	94	PHE	5.2
1	D	30	LYS	5.2
2	E	229	MET	5.2
1	D	144	GLU	5.1
2	E	82	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
2	E	92	PHE	5.1
2	E	93	PHE	5.1
2	E	230	LYS	5.0
1	D	145	TYR	5.0
1	D	148	PRO	5.0
1	D	122	TRP	4.9
2	E	207	ILE	4.8
1	A	406	ALA	4.8
2	E	81	TYR	4.7
1	D	13	PRO	4.7
2	E	53	VAL	4.5
2	E	116	GLY	4.5
2	B	4	GLU	4.5
2	E	111	VAL	4.5
2	E	23	ILE	4.4
1	D	291	CYS	4.4
2	E	54	VAL	4.4
1	D	247	GLU	4.3
1	D	276	LYS	4.3
2	E	232	LYS	4.3
1	D	2	GLU	4.3
1	D	12	GLY	4.3
1	D	417	TRP	4.3
2	E	234	ILE	4.1
1	D	110	LYS	4.0
1	A	276	LYS	4.0
2	E	109	GLU	3.9
2	E	21	PRO	3.9
1	D	1	SER	3.9
1	A	417	TRP	3.8
2	E	231	ASN	3.8
1	D	207	MET	3.8
1	D	68	VAL	3.7
2	E	107	VAL	3.7
1	D	219	CYS	3.7
2	E	40	VAL	3.7
2	E	110	ARG	3.7
2	E	205	GLU	3.7
2	E	46	GLU	3.6
1	D	292	ILE	3.6
1	D	40	MET	3.6
2	E	95	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	126	LEU	3.6
2	E	164	ASP	3.6
1	A	411	LEU	3.5
1	D	357	PHE	3.5
2	E	211	CYS	3.5
1	D	66	GLY	3.5
2	B	5	GLY	3.5
2	E	123	LYS	3.5
2	E	209	LYS	3.5
1	D	81	TYR	3.5
1	D	107	TYR	3.5
1	D	36	LYS	3.5
1	D	163	GLY	3.5
1	D	251	GLU	3.4
1	A	414	ARG	3.4
2	E	101	ASP	3.4
1	D	162	ILE	3.4
1	D	72	GLY	3.4
1	A	404	PRO	3.4
1	D	102	PRO	3.3
2	E	49	ASP	3.3
1	D	80	ARG	3.3
2	E	35	VAL	3.3
1	D	11	LYS	3.3
2	E	72	ASP	3.3
2	E	17	ASP	3.2
2	E	32	TYR	3.2
1	D	248	ALA	3.1
2	E	298	THR	3.1
2	E	43	ARG	3.1
2	E	208	ARG	3.1
1	D	53	ILE	3.1
2	E	239	GLU	3.1
1	A	86	GLU	3.0
2	E	77	TYR	3.0
1	D	59	LYS	3.0
2	E	15	PHE	3.0
2	E	135	GLN	3.0
1	D	115	LEU	2.9
1	D	9	LEU	2.9
1	D	84	LEU	2.9
1	D	25	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	317	PHE	2.9
2	E	28	GLY	2.9
1	D	123	GLY	2.9
1	D	31	ALA	2.9
1	D	181	CYS	2.9
2	E	8	THR	2.9
2	E	56	PHE	2.8
1	D	91	VAL	2.8
1	D	318	VAL	2.8
1	D	24	THR	2.8
2	E	118	THR	2.8
2	E	160	GLU	2.8
2	E	96	ASP	2.8
1	D	178	PRO	2.8
1	D	138	PHE	2.8
2	E	244	CYS	2.8
2	E	163	THR	2.8
1	D	21	ILE	2.8
2	E	158	LEU	2.8
2	E	99	LYS	2.7
1	D	44	ALA	2.7
1	D	5	LEU	2.7
2	E	98	SER	2.7
2	E	14	TYR	2.7
1	D	18	VAL	2.7
1	D	34	GLU	2.7
2	E	36	VAL	2.7
1	D	45	ARG	2.7
1	D	32	ALA	2.7
1	D	114	GLY	2.7
1	D	41	PRO	2.6
1	D	85	GLY	2.6
2	E	236	VAL	2.6
1	D	160	PHE	2.6
2	E	221	PRO	2.6
2	E	297	PRO	2.6
2	E	245	GLY	2.6
2	E	50	VAL	2.6
2	E	25	LYS	2.6
1	D	87	GLN	2.6
2	E	108	GLN	2.6
1	D	119	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	97	GLU	2.6
2	E	27	TYR	2.5
1	D	139	LEU	2.5
1	A	416	MET	2.5
1	D	258	ILE	2.5
1	D	106	PHE	2.5
1	D	205	ARG	2.5
2	E	44	VAL	2.5
1	D	140	GLY	2.5
2	E	114	PRO	2.5
2	E	76	LYS	2.5
2	E	206	ALA	2.5
1	D	224	VAL	2.5
1	D	124	SER	2.5
1	D	303	ASP	2.5
1	D	97	MET	2.4
1	D	108	SER	2.4
1	D	92	GLU	2.4
1	D	254	SER	2.4
2	E	339	GLU	2.4
2	E	65	TYR	2.4
2	E	161	TYR	2.4
2	E	302	TYR	2.4
1	D	245	ASP	2.4
2	E	210	THR	2.4
1	D	262	VAL	2.4
2	E	309	ALA	2.4
1	D	56	LYS	2.4
1	D	153	LEU	2.4
1	D	278	LEU	2.4
1	D	334	GLU	2.4
1	D	201	ASP	2.3
2	E	63	SER	2.3
1	D	137	ILE	2.3
1	D	93	HIS	2.3
2	E	335	LEU	2.3
1	D	134	GLY	2.3
1	D	275	GLY	2.3
1	D	28	MET	2.3
1	D	46	GLY	2.3
2	E	90	VAL	2.3
1	D	105	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	138	ILE	2.3
1	D	10	GLU	2.3
1	D	277	GLU	2.3
2	E	148	SER	2.2
1	D	121	LYS	2.2
1	D	38	VAL	2.2
2	E	314	ALA	2.2
1	D	146	LEU	2.2
2	E	214	PRO	2.2
2	E	94	VAL	2.2
2	E	213	ILE	2.2
1	D	203	LEU	2.2
2	E	227	PRO	2.2
2	E	252	PRO	2.2
1	A	407	TYR	2.2
1	D	43	GLY	2.2
2	E	47	SER	2.2
1	D	289	MET	2.2
1	D	35	GLY	2.2
2	E	31	LYS	2.2
1	A	292	ILE	2.2
1	D	99	ILE	2.2
2	E	146	ASP	2.1
2	E	240	LYS	2.1
2	E	140	CYS	2.1
2	E	41	ILE	2.1
1	D	57	ASP	2.1
1	D	125	GLY	2.1
2	E	181	MET	2.1
2	E	70	LEU	2.1
1	D	274	ASP	2.1
1	D	223	CYS	2.1
2	E	288	TRP	2.1
1	D	83	ASP	2.1
1	D	117	ASP	2.1
2	E	102	ASP	2.1
2	E	30	TRP	2.0
2	E	137	TRP	2.0
1	D	88	ILE	2.0
2	E	256	LEU	2.0
1	D	131	GLY	2.0
2	E	149	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	157	GLU	2.0
1	D	142	ARG	2.0
1	D	17	PHE	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, 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
3	SRM	E	570	63/63	0.84	0.42	4.64	11,15,19,22	0
3	SRM	D	580	63/63	0.81	0.42	2.92	40,56,68,71	0
4	SF4	D	575	8/8	0.94	0.26	2.39	6,7,7,8	0
4	SF4	E	585	8/8	0.89	0.31	2.16	32,34,36,40	0
4	SF4	D	576	8/8	0.92	0.19	0.47	7,10,10,10	0
5	GOL	A	590	6/6	0.94	0.11	0.21	25,30,37,42	0
3	SRM	A	580	63/63	0.96	0.11	-0.02	16,23,33,41	0
4	SF4	E	586	8/8	0.96	0.16	-0.69	20,22,24,24	0
4	SF4	A	576	8/8	0.95	0.10	-1.32	4,5,6,6	0
3	SRM	B	570	63/63	0.97	0.09	-1.39	6,8,13,16	0
4	SF4	B	586	8/8	0.99	0.09	-1.57	19,22,24,25	0
4	SF4	B	585	8/8	0.98	0.06	-2.53	16,19,20,36	0
4	SF4	A	575	8/8	0.97	0.05	-3.53	7,8,10,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.