



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 06:21 PM EDT

PDB ID : 3MMA  
Title : Dissimilatory sulfite reductase phosphate complex  
Authors : Parey, K.; Warkentin, E.; Kroneck, P.M.H.; Ermler, U.  
Deposited on : unknown  
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

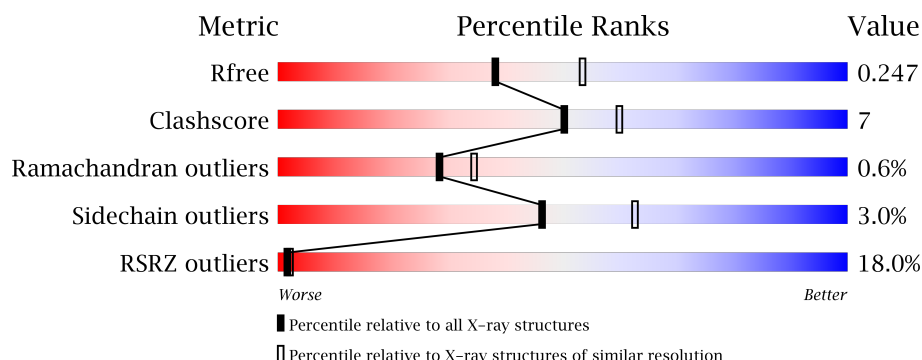
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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>7%</div> <div>86%</div> <div>13%</div> </div>
1	D	418	<div> <div>31%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	B	366	<div> <div>5%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
2	E	366	<div> <div>28%</div> <div>79%</div> <div>18%</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	E	585	-	-	X	-
5	PO4	A	590	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12960 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.

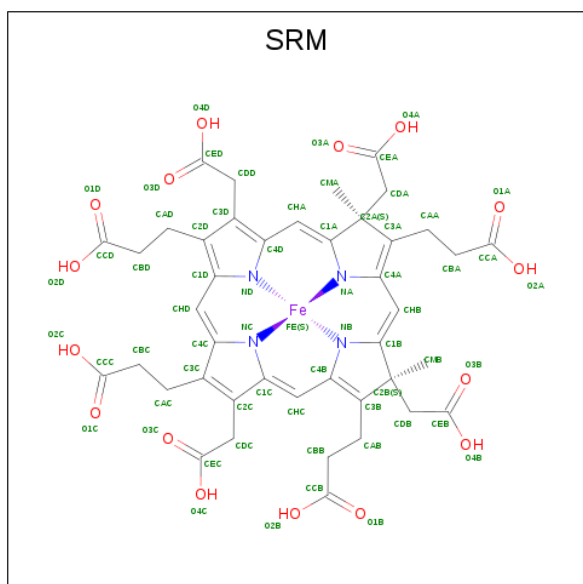
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

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.

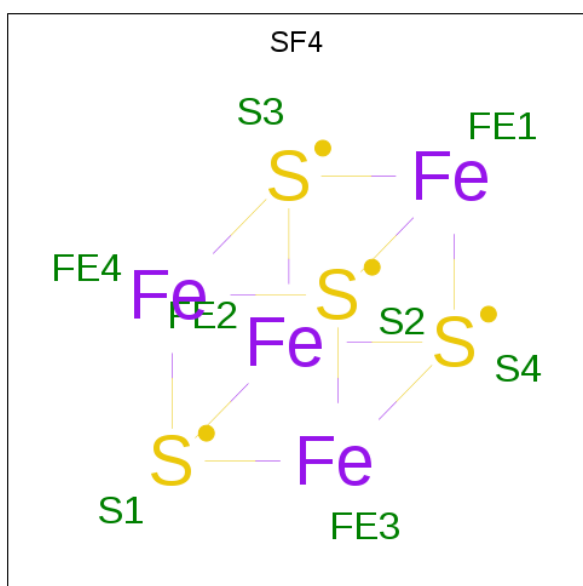
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			
2	E	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			

- 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 PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

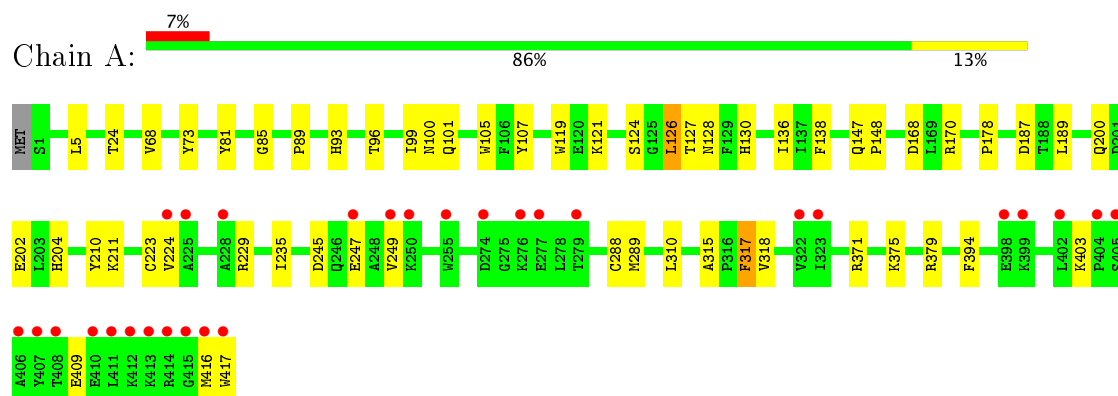
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	78	Total	O	0	0
			78	78		
6	B	84	Total	O	0	0
			84	84		
6	D	11	Total	O	0	0
			11	11		
6	E	6	Total	O	0	0
			6	6		

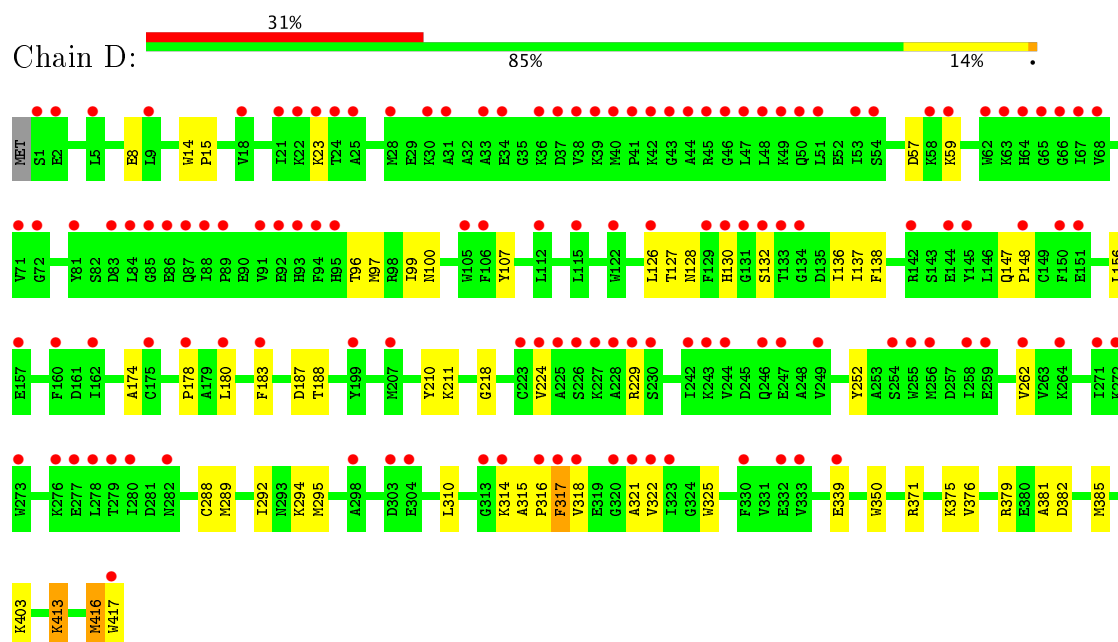
### 3 Residue-property plots [i](#)

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

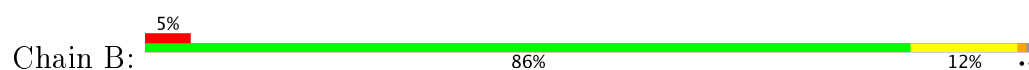
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

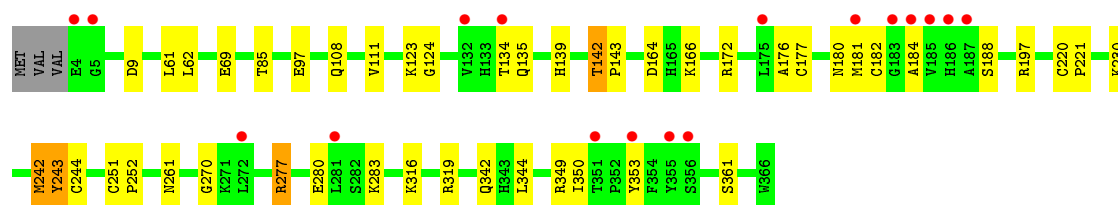


- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

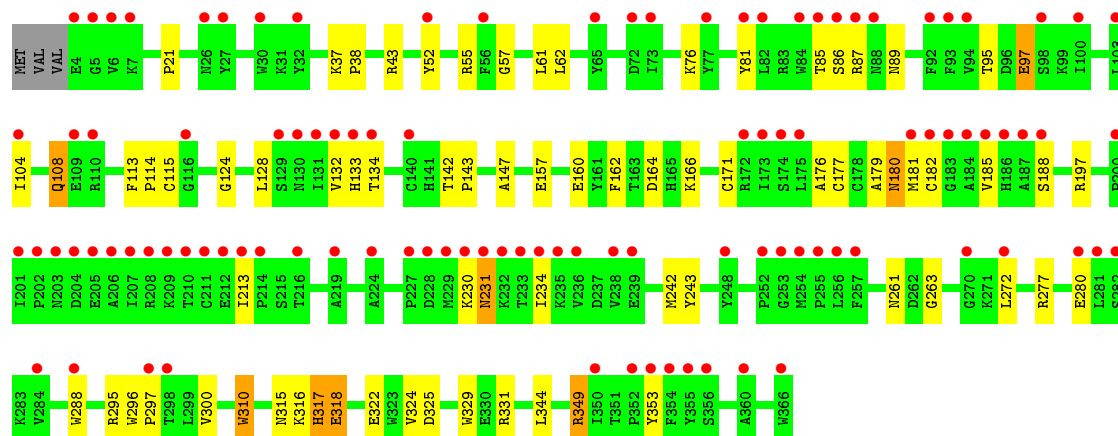
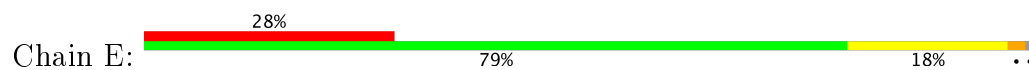


- Molecule 2: Sulfite reductase, dissimilatory-type subunit beta





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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.60Å 68.90Å 145.10Å 90.00° 107.50° 90.00°	Depositor
Resolution (Å)	48.34 – 2.30 48.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.34-2.30) 98.8 (48.33-2.30)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.81 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, $R_{free}$	0.192 , 0.236 0.211 , 0.247	Depositor DCC
$R_{free}$ test set	3928 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, PO4, 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	0.55	1/3416 (0.0%)	0.63	0/4610
1	D	0.42	1/3416 (0.0%)	0.53	0/4610
2	B	0.54	0/2984	0.65	1/4058 (0.0%)
2	E	0.40	0/2984	0.55	0/4058
All	All	0.48	2/12800 (0.0%)	0.59	1/17336 (0.0%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	CYS	CB-SG	8.13	1.96	1.82
1	D	23	LYS	CD-CE	5.95	1.66	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	277	ARG	NE-CZ-NH1	5.13	122.87	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	PHE	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	3329	0	3276	45	0
1	D	3329	0	3276	44	0
2	B	2901	0	2837	37	0
2	E	2901	0	2838	53	0
3	A	63	0	34	12	0
3	B	63	0	34	6	0
3	D	63	0	34	6	0
3	E	63	0	34	11	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
4	D	16	0	0	1	0
4	E	16	0	0	2	0
5	A	5	0	0	2	0
6	A	78	0	0	1	0
6	B	84	0	0	1	0
6	D	11	0	0	2	0
6	E	6	0	0	0	0
All	All	12960	0	12363	167	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 7.

All (167) 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)
3:E:570:SRM:HBD2	3:E:570:SRM:HDD2	1.33	1.07
1:A:403:LYS:H	2:E:261:ASN:HD21	1.07	0.97
2:E:230:LYS:HB2	2:E:231:ASN:HB2	1.48	0.95
1:D:317:PHE:HD2	2:E:180:ASN:HB3	1.35	0.88
2:E:177:CYS:HB2	4:E:585:SF4:S3	2.14	0.88
2:E:157:GLU:HG3	2:E:300:VAL:HG11	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:570:SRM:HDD2	3:E:570:SRM:CBD	2.03	0.88
2:B:261:ASN:HD21	1:D:403:LYS:H	1.21	0.87
1:D:128:ASN:HB2	1:D:137:ILE:HB	1.59	0.84
1:D:317:PHE:CD2	2:E:180:ASN:HB3	2.14	0.83
2:E:55:ARG:HH22	3:E:570:SRM:HBA2	1.45	0.80
2:E:230:LYS:CB	2:E:231:ASN:HB2	2.12	0.79
2:E:157:GLU:HG3	2:E:300:VAL:CG1	2.14	0.78
2:E:197:ARG:HH21	2:E:261:ASN:HD22	1.32	0.77
2:E:230:LYS:HB2	2:E:231:ASN:CB	2.14	0.77
2:E:52:TYR:CE1	2:E:97:GLU:HB3	2.18	0.77
2:E:134:THR:HG21	2:E:182:CYS:HB2	1.65	0.77
2:B:124:GLY:HA3	2:B:316:LYS:HD3	1.67	0.75
1:A:107:TYR:OH	1:A:130:HIS:HE1	1.70	0.74
1:A:317:PHE:CD2	2:B:180:ASN:HB3	2.22	0.74
2:E:85:THR:HB	3:E:570:SRM:HAB2	1.69	0.73
1:A:229:ARG:HD3	2:B:184:ALA:HB2	1.69	0.72
1:D:178:PRO:HG3	1:D:187:ASP:HA	1.72	0.69
1:A:317:PHE:HD2	2:B:180:ASN:HB3	1.60	0.67
1:A:379:ARG:HH11	1:A:379:ARG:HG3	1.60	0.66
1:D:379:ARG:HG3	1:D:379:ARG:HH11	1.61	0.65
2:E:86:SER:OG	3:E:570:SRM:HAB1	1.96	0.65
2:B:69:GLU:HG2	6:B:381:HOH:O	1.96	0.65
2:E:124:GLY:HA3	2:E:316:LYS:HD2	1.79	0.64
1:D:147:GLN:HB3	1:D:148:PRO:HD3	1.79	0.64
1:D:218:GLY:HA3	4:D:575:SF4:S2	2.39	0.64
1:A:96:THR:HG23	2:B:139:HIS:CE1	2.33	0.63
1:A:128:ASN:ND2	2:B:135:GLN:HE22	1.97	0.63
1:D:107:TYR:OH	1:D:130:HIS:HE1	1.83	0.61
2:E:230:LYS:CA	2:E:231:ASN:HB2	2.31	0.61
1:A:416:MET:O	1:A:417:TRP:HB2	2.00	0.60
2:B:261:ASN:HD21	1:D:403:LYS:N	1.94	0.60
1:A:403:LYS:N	2:E:261:ASN:HD21	1.90	0.60
2:E:57:GLY:HA2	2:E:89:ASN:ND2	2.17	0.60
1:D:99:ILE:HB	1:D:136:ILE:HB	1.83	0.60
1:A:128:ASN:HD21	2:B:135:GLN:HE22	1.49	0.59
1:D:132:SER:N	3:D:580:SRM:HBB1	2.17	0.59
1:A:394:PHE:HE2	2:E:179:ALA:HB1	1.68	0.59
2:B:350:ILE:O	2:E:349:ARG:NH2	2.28	0.59
2:E:272:LEU:HB2	3:E:570:SRM:CCC	2.33	0.59
1:A:315:ALA:HB3	3:A:580:SRM:HBD1	1.84	0.58
1:A:371:ARG:O	1:A:375:LYS:HD3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:570:SRM:HBA1	3:E:570:SRM:CHB	2.31	0.56
3:D:580:SRM:HMB1	3:D:580:SRM:HBB2	1.87	0.56
1:D:211:LYS:NZ	3:D:580:SRM:HAD1	2.21	0.55
1:D:317:PHE:HE2	2:E:180:ASN:HD22	1.54	0.55
1:A:119:TRP:CH2	1:A:138:PHE:HB3	2.41	0.55
2:E:37:LYS:HB2	2:E:38:PRO:CD	2.36	0.55
2:B:197:ARG:HH21	2:B:261:ASN:HD22	1.55	0.55
1:A:168:ASP:OD1	1:A:170:ARG:HD3	2.06	0.55
2:B:277:ARG:NH2	2:B:280:GLU:OE1	2.38	0.55
3:A:580:SRM:CMB	3:A:580:SRM:CBB	2.85	0.55
1:A:107:TYR:OH	1:A:130:HIS:CE1	2.58	0.54
3:A:580:SRM:C4C	2:B:182:CYS:HA	2.36	0.54
1:A:394:PHE:CE2	2:E:179:ALA:HB1	2.41	0.54
2:E:108:GLN:NE2	2:E:113:PHE:O	2.40	0.53
1:A:170:ARG:HH12	5:A:590:PO4:P	2.32	0.53
1:D:15:PRO:HD3	2:E:114:PRO:HD3	1.90	0.53
1:A:99:ILE:HB	1:A:136:ILE:HB	1.89	0.53
1:D:156:LEU:HD12	6:D:428:HOH:O	2.08	0.53
1:A:379:ARG:HH11	1:A:379:ARG:CG	2.21	0.52
1:D:262:VAL:HG22	1:D:294:LYS:HG3	1.90	0.52
1:D:413:LYS:HG2	6:D:420:HOH:O	2.08	0.52
2:E:128:LEU:O	2:E:162:PHE:HA	2.10	0.52
2:E:181:MET:HG2	2:E:185:VAL:HB	1.92	0.52
1:A:211:LYS:NZ	5:A:590:PO4:O1	2.30	0.52
2:E:134:THR:HB	4:E:585:SF4:S4	2.50	0.51
2:E:87:ARG:HG3	3:E:570:SRM:HBB2	1.93	0.51
2:E:133:HIS:HB2	2:E:147:ALA:HB1	1.92	0.51
1:A:229:ARG:HG2	3:A:580:SRM:HCD1	1.92	0.51
1:D:14:TRP:CD2	1:D:15:PRO:HD2	2.45	0.51
2:E:104:ILE:HG23	2:E:115:CYS:HB2	1.93	0.51
2:E:324:VAL:HG11	2:E:329:TRP:CE2	2.45	0.50
2:B:85:THR:HB	3:B:570:SRM:CAB	2.41	0.50
2:B:176:ALA:HB1	2:B:181:MET:HA	1.94	0.50
1:D:229:ARG:HG2	3:D:580:SRM:HCD1	1.93	0.49
1:D:180:LEU:O	2:E:43:ARG:HD3	2.12	0.49
1:A:211:LYS:HZ1	3:A:580:SRM:HAD1	1.77	0.49
2:B:172:ARG:HH21	3:B:570:SRM:C2C	2.25	0.49
3:A:580:SRM:HHB	3:A:580:SRM:HBA1	1.95	0.49
1:D:8:GLU:O	2:E:295:ARG:NH2	2.44	0.49
1:D:379:ARG:CG	1:D:379:ARG:HH11	2.24	0.48
1:A:24:THR:HG21	1:A:126:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:322:GLU:O	2:E:325:ASP:HB2	2.12	0.48
1:D:288:CYS:O	1:D:289:MET:HB2	2.13	0.48
2:E:315:ASN:O	2:E:318:GLU:HB3	2.14	0.48
1:A:245:ASP:OD1	1:A:247:GLU:HG2	2.14	0.48
3:E:570:SRM:CHB	3:E:570:SRM:CBA	2.91	0.48
2:B:353:TYR:HA	2:E:353:TYR:HA	1.96	0.47
2:E:316:LYS:O	2:E:317:HIS:HB2	2.14	0.47
1:D:416:MET:O	1:D:417:TRP:HB3	2.14	0.47
2:E:230:LYS:HB2	2:E:231:ASN:CG	2.34	0.47
1:A:147:GLN:HB3	1:A:148:PRO:HD3	1.95	0.47
2:E:164:ASP:HB3	2:E:166:LYS:HG3	1.96	0.47
1:A:288:CYS:O	1:A:289:MET:HB2	2.14	0.47
1:A:317:PHE:CE2	2:B:180:ASN:HB3	2.49	0.47
1:A:168:ASP:HB2	1:A:202:GLU:O	2.15	0.47
2:B:142:THR:N	2:B:143:PRO:CD	2.77	0.46
2:E:142:THR:N	2:E:143:PRO:HD3	2.30	0.46
1:A:245:ASP:O	1:A:249:VAL:HG23	2.15	0.46
1:D:97:MET:HB2	1:D:138:PHE:HB2	1.96	0.46
2:E:57:GLY:HA2	2:E:89:ASN:HD22	1.80	0.45
1:A:200:GLN:NE2	1:A:204:HIS:NE2	2.65	0.45
1:D:107:TYR:OH	1:D:130:HIS:CE1	2.67	0.45
3:A:580:SRM:HHB	3:A:580:SRM:CBA	2.47	0.45
1:D:315:ALA:HB1	1:D:316:PRO:CD	2.47	0.45
3:A:580:SRM:CEB	2:B:134:THR:HG22	2.46	0.45
1:A:121:LYS:NZ	6:A:477:HOH:O	2.49	0.45
2:E:263:GLY:HA3	2:E:288:TRP:NE1	2.31	0.45
2:B:124:GLY:HA3	2:B:316:LYS:CD	2.44	0.44
1:D:339:GLU:OE2	1:D:379:ARG:NH2	2.50	0.44
1:D:314:LYS:HG2	1:D:322:VAL:HB	1.99	0.44
2:B:85:THR:HB	3:B:570:SRM:HAB1	1.99	0.44
1:D:252:TYR:CE2	1:D:295:MET:HB3	2.53	0.44
1:A:127:THR:O	2:B:61:LEU:HD12	2.17	0.44
1:D:316:PRO:HA	1:D:321:ALA:N	2.32	0.44
2:B:242:MET:SD	2:B:244:CYS:HB3	2.58	0.44
3:B:570:SRM:HDD2	3:B:570:SRM:HBD2	1.99	0.44
2:B:85:THR:HB	3:B:570:SRM:HAB2	1.99	0.44
2:B:69:GLU:OE2	2:B:111:VAL:HG12	2.17	0.43
1:D:57:ASP:HB3	1:D:59:LYS:HG2	1.99	0.43
1:A:379:ARG:CG	1:A:379:ARG:NH1	2.81	0.43
3:A:580:SRM:HMB3	3:A:580:SRM:HBB2	2.00	0.43
1:D:310:LEU:HA	1:D:325:TRP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLN:HE21	2:B:9:ASP:HA	1.83	0.43
2:E:21:PRO:HD3	2:E:81:TYR:CE1	2.55	0.42
1:A:211:LYS:NZ	3:A:580:SRM:HAD1	2.35	0.42
1:D:174:ALA:HB1	1:D:188:THR:HB	2.00	0.42
2:E:176:ALA:HB1	2:E:181:MET:HA	2.01	0.42
2:B:342:GLN:HB3	1:D:381:ALA:HB2	2.02	0.42
1:D:127:THR:O	2:E:61:LEU:HD12	2.20	0.42
2:B:164:ASP:HB3	2:B:166:LYS:HG3	2.01	0.42
2:E:296:TRP:N	2:E:297:PRO:HD3	2.34	0.42
3:A:580:SRM:CMB	3:A:580:SRM:HBB2	2.48	0.42
1:A:85:GLY:O	1:A:89:PRO:HA	2.20	0.42
2:B:188:SER:N	2:B:270:GLY:HA3	2.35	0.42
1:D:132:SER:H	3:D:580:SRM:HBB1	1.83	0.42
1:D:382:ASP:O	1:D:385:MET:HG3	2.20	0.41
2:E:171:CYS:HB2	2:E:310:TRP:CH2	2.55	0.41
3:E:570:SRM:CDD	3:E:570:SRM:CBD	2.86	0.41
1:A:73:TYR:CD1	1:A:204:HIS:HB3	2.55	0.41
1:D:315:ALA:HB3	3:D:580:SRM:HBD1	2.01	0.41
2:B:123:LYS:HD2	2:B:123:LYS:HA	1.92	0.41
2:B:251:CYS:HA	2:B:252:PRO:HD2	1.88	0.41
1:A:124:SER:OG	1:A:126:LEU:HB2	2.21	0.41
1:D:183:PHE:CE1	1:D:292:ILE:HG22	2.56	0.41
1:A:101:GLN:HG3	1:A:105:TRP:CD1	2.55	0.41
3:E:570:SRM:HCD1	3:E:570:SRM:HAC2	1.66	0.41
1:A:235:ILE:HD12	1:A:310:LEU:HD22	2.01	0.41
2:B:242:MET:C	2:B:243:TYR:CG	2.94	0.41
2:B:220:CYS:HA	2:B:221:PRO:HD3	1.91	0.40
2:E:213:ILE:HG23	2:E:234:ILE:HG12	2.03	0.40
2:E:277:ARG:NH2	2:E:280:GLU:OE1	2.50	0.40
1:A:178:PRO:HG3	1:A:187:ASP:HA	2.02	0.40
2:B:319:ARG:HH22	3:B:570:SRM:CCC	2.34	0.40
1:A:119:TRP:CZ3	1:A:138:PHE:HB3	2.56	0.40
3:A:580:SRM:HAD1	3:A:580:SRM:O4D	2.22	0.40
2:E:197:ARG:NH2	2:E:261:ASN:HD22	2.09	0.40
1:A:81:TYR:CE2	1:A:93:HIS:CD2	3.10	0.40
2:B:342:GLN:CD	1:D:371:ARG:HG3	2.42	0.40
1:D:127:THR:HA	1:D:137:ILE:O	2.22	0.40
1:D:350:TRP:CG	1:D:376:VAL:HG21	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	51	63
1	D	415/418 (99%)	393 (95%)	21 (5%)	1 (0%)	51	63
2	B	361/366 (99%)	343 (95%)	16 (4%)	2 (1%)	28	34
2	E	361/366 (99%)	331 (92%)	25 (7%)	5 (1%)	13	13
All	All	1552/1568 (99%)	1469 (95%)	74 (5%)	9 (1%)	28	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	VAL
2	E	317	HIS
1	D	318	VAL
2	E	76	LYS
2	E	231	ASN
2	E	160	GLU
2	B	361	SER
2	E	318	GLU
2	B	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%)	345 (98%)	8 (2%)	56	73
1	D	353/354 (100%)	344 (98%)	9 (2%)	53	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	314/317 (99%)	304 (97%)	10 (3%)	44	60
2	E	314/317 (99%)	301 (96%)	13 (4%)	35	48
All	All	1334/1342 (99%)	1294 (97%)	40 (3%)	46	63

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	68	VAL
1	A	100	ASN
1	A	126	LEU
1	A	189	LEU
1	A	210	TYR
1	A	224	VAL
1	A	409	GLU
2	B	62	LEU
2	B	97	GLU
2	B	108	GLN
2	B	177	CYS
2	B	230	LYS
2	B	242	MET
2	B	243	TYR
2	B	283	LYS
2	B	344	LEU
2	B	349	ARG
1	D	96	THR
1	D	100	ASN
1	D	126	LEU
1	D	210	TYR
1	D	224	VAL
1	D	317	PHE
1	D	375	LYS
1	D	413	LYS
1	D	416	MET
2	E	62	LEU
2	E	95	THR
2	E	97	GLU
2	E	108	GLN
2	E	132	VAL
2	E	180	ASN
2	E	188	SER

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Mol	Chain	Res	Type
2	E	242	MET
2	E	243	TYR
2	E	310	TRP
2	E	331	ARG
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	100	ASN
1	A	128	ASN
1	A	130	HIS
1	A	200	GLN
2	B	89	ASN
2	B	261	ASN
1	D	93	HIS
1	D	100	ASN
1	D	130	HIS
1	D	200	GLN
2	E	89	ASN
2	E	108	GLN
2	E	231	ASN
2	E	261	ASN
2	E	363	GLN

### 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	34,70,70	1.93	7 (20%)	34,112,112	3.83	18 (52%)
5	PO4	A	590	-	4,4,4	0.92	0	6,6,6	0.82	0
3	SRM	B	570	1	34,70,70	2.49	10 (29%)	34,112,112	4.13	19 (55%)
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	-	34,70,70	1.95	9 (26%)	34,112,112	3.33	13 (38%)
3	SRM	E	570	-	34,70,70	2.73	10 (29%)	34,112,112	3.95	21 (61%)
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	-	1/22/126/126	0/0/8/8
5	PO4	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	-	0/0/48/48	0/6/5/5
3	SRM	D	580	-	-	0/22/126/126	0/0/8/8
3	SRM	E	570	-	-	0/22/126/126	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	E	570	SRM	C4C-NC	-7.09	1.28	1.36
3	E	570	SRM	C1C-NC	-6.71	1.28	1.36
3	B	570	SRM	C4C-NC	-6.08	1.29	1.36
3	B	570	SRM	C4A-NA	-5.80	1.28	1.39
3	E	570	SRM	C4A-NA	-5.64	1.28	1.39
3	E	570	SRM	C1B-NB	-5.16	1.29	1.38
3	B	570	SRM	C1C-NC	-4.81	1.31	1.36
3	B	570	SRM	C1B-NB	-4.41	1.30	1.38
3	D	580	SRM	C4A-NA	-3.11	1.33	1.39
3	A	580	SRM	C4A-NA	-3.09	1.33	1.39
3	B	570	SRM	CDA-C2A	-2.77	1.52	1.56
3	A	580	SRM	C4C-NC	-2.74	1.33	1.36
3	E	570	SRM	C4B-NB	-2.72	1.34	1.39
3	D	580	SRM	C4C-NC	-2.54	1.33	1.36
3	E	570	SRM	CHC-C4B	-2.31	1.34	1.39
3	D	580	SRM	C1A-NA	-2.20	1.34	1.38
3	A	580	SRM	C1C-NC	-2.18	1.34	1.36
3	D	580	SRM	C4B-NB	-2.17	1.35	1.39
3	E	570	SRM	CHB-C4A	-2.14	1.34	1.39
3	D	580	SRM	C1C-NC	-2.07	1.34	1.36
3	B	570	SRM	C1D-CHD	-2.02	1.34	1.40
3	B	570	SRM	CAD-C2D	2.02	1.55	1.52
3	E	570	SRM	CHA-C1A	2.16	1.39	1.36
3	B	570	SRM	CAA-C3A	3.00	1.56	1.51
3	D	580	SRM	FE-NA	3.51	2.09	1.95
3	D	580	SRM	FE-NB	3.55	2.09	1.95
3	A	580	SRM	FE-NB	3.62	2.10	1.95
3	A	580	SRM	C3C-C2C	3.84	1.49	1.37
3	A	580	SRM	FE-NA	4.10	2.11	1.95
3	D	580	SRM	C3C-C2C	4.15	1.50	1.37
3	B	570	SRM	C3C-C2C	4.48	1.50	1.37
3	E	570	SRM	C3C-C2C	4.64	1.51	1.37
3	B	570	SRM	C3D-C2D	5.42	1.52	1.39
3	E	570	SRM	C3D-C2D	5.76	1.53	1.39
3	A	580	SRM	C3D-C2D	6.19	1.54	1.39
3	D	580	SRM	C3D-C2D	6.27	1.54	1.39

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	580	SRM	CAB-C3B-C2B	-15.26	106.27	123.52
3	B	570	SRM	CAA-C3A-C2A	-12.23	109.69	123.52
3	D	580	SRM	CAB-C3B-C2B	-11.94	110.02	123.52
3	E	570	SRM	CAA-C3A-C2A	-10.71	111.41	123.52
3	E	570	SRM	CDC-C2C-C1C	-9.58	112.92	127.39
3	A	580	SRM	CAD-C2D-C3D	-7.78	110.02	129.38
3	B	570	SRM	CEC-CDC-C2C	-6.69	103.11	116.14
3	D	580	SRM	CDD-C3D-C2D	-6.06	115.55	126.48
3	B	570	SRM	CBC-CAC-C3C	-5.87	101.28	112.47
3	E	570	SRM	C4A-NA-C1A	-5.83	102.44	106.37
3	A	580	SRM	CAA-C3A-C2A	-5.44	117.38	123.52
3	E	570	SRM	CAC-C3C-C2C	-5.37	116.02	129.38
3	D	580	SRM	CAD-C2D-C3D	-5.23	116.35	129.38
3	E	570	SRM	CDC-C2C-C3C	-5.20	117.11	126.48
3	B	570	SRM	C4D-CHA-C1A	-5.20	119.83	130.12
3	D	580	SRM	CAA-C3A-C2A	-5.15	117.69	123.52
3	E	570	SRM	C4D-CHA-C1A	-5.14	119.94	130.12
3	B	570	SRM	C4A-NA-C1A	-4.64	103.24	106.37
3	E	570	SRM	CAD-C2D-C3D	-4.61	117.90	129.38
3	A	580	SRM	CDD-C3D-C2D	-4.57	118.24	126.48
3	B	570	SRM	C3B-C2B-C1B	-4.45	93.37	101.25
3	B	570	SRM	CAC-C3C-C2C	-4.38	118.48	129.38
3	D	580	SRM	CDD-C3D-C4D	-4.25	120.92	127.36
3	E	570	SRM	CHB-C4A-C3A	-4.17	116.01	125.47
3	E	570	SRM	CDD-C3D-C2D	-3.98	119.31	126.48
3	B	570	SRM	CDC-C2C-C3C	-3.94	119.37	126.48
3	E	570	SRM	C3B-C2B-C1B	-3.72	94.66	101.25
3	E	570	SRM	CDD-C3D-C4D	-3.72	121.73	127.36
3	D	580	SRM	C4D-CHA-C1A	-3.69	122.80	130.12
3	A	580	SRM	C3A-C2A-C1A	-3.63	94.83	101.25
3	B	570	SRM	CHB-C4A-C3A	-3.58	117.35	125.47
3	A	580	SRM	CAC-CBC-CCC	-3.51	106.66	112.66
3	B	570	SRM	CDC-C2C-C1C	-3.37	122.31	127.39
3	A	580	SRM	CDD-C3D-C4D	-3.22	122.48	127.36
3	E	570	SRM	CEC-CDC-C2C	-3.12	110.08	116.14
3	D	580	SRM	C3A-C2A-C1A	-3.01	95.93	101.25
3	D	580	SRM	CHA-C1A-NA	-2.80	119.77	124.18
3	B	570	SRM	CAB-C3B-C2B	-2.69	120.48	123.52
3	B	570	SRM	CAD-C2D-C3D	-2.63	122.83	129.38
3	A	580	SRM	CAD-CBD-CCD	-2.56	108.28	112.66
3	D	580	SRM	C3B-C2B-C1B	-2.56	96.72	101.25
3	D	580	SRM	C4B-NB-C1B	-2.52	104.67	106.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	580	SRM	C3B-C2B-C1B	-2.42	96.97	101.25
3	A	580	SRM	C3A-C4A-NA	-2.23	107.57	110.12
3	A	580	SRM	C4D-CHA-C1A	-2.20	125.75	130.12
3	D	580	SRM	CHB-C1B-NB	-2.20	120.72	124.18
3	E	570	SRM	C2B-C1B-CHB	-2.14	116.56	124.10
3	E	570	SRM	C2A-C1A-CHA	-2.12	116.64	124.10
3	E	570	SRM	CBC-CAC-C3C	-2.01	108.63	112.47
3	B	570	SRM	CHC-C4B-NB	2.02	127.59	123.80
3	E	570	SRM	CAB-CBB-CCB	2.04	116.15	112.66
3	A	580	SRM	CBC-CAC-C3C	2.15	116.57	112.47
3	E	570	SRM	CAA-CBA-CCA	2.17	116.36	112.66
3	E	570	SRM	C2B-CDB-CEB	2.32	118.83	115.39
3	E	570	SRM	CAB-C3B-C2B	2.34	126.17	123.52
3	A	580	SRM	C3B-C4B-NB	2.39	112.86	110.12
3	A	580	SRM	CED-CDD-C3D	2.59	121.19	116.14
3	E	570	SRM	CED-CDD-C3D	2.60	121.22	116.14
3	B	570	SRM	CED-CDD-C3D	2.91	121.81	116.14
3	A	580	SRM	C2A-CDA-CEA	2.99	119.81	115.39
3	A	580	SRM	CDC-C2C-C1C	3.12	132.11	127.39
3	D	580	SRM	C3B-C4B-NB	3.25	113.83	110.12
3	A	580	SRM	CBD-CAD-C2D	3.79	119.74	112.48
3	B	570	SRM	CAA-CBA-CCA	4.01	119.52	112.66
3	B	570	SRM	C2B-CDB-CEB	5.37	123.34	115.39
3	A	580	SRM	C4A-NA-C1A	5.66	110.19	106.37
3	B	570	SRM	CAB-CBB-CCB	5.78	122.53	112.66
3	B	570	SRM	CBD-CAD-C2D	6.32	124.57	112.48
3	D	580	SRM	C4A-NA-C1A	6.75	110.92	106.37
3	B	570	SRM	C3A-C4A-NA	7.20	118.35	110.12
3	E	570	SRM	C3A-C4A-NA	8.31	119.62	110.12

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	580	SRM	C3D-C2D-CAD-CBD

There are no ring outliers.

7 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	580	SRM	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	590	PO4	2	0
3	B	570	SRM	6	0
4	D	575	SF4	1	0
3	D	580	SRM	6	0
3	E	570	SRM	11	0
4	E	585	SF4	2	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%)	0.39	29 (6%)	17 23	12, 19, 35, 78	0
1	D	417/418 (99%)	1.49	131 (31%)	0 0	13, 23, 36, 54	0
2	B	363/366 (99%)	0.35	17 (4%)	32 39	11, 18, 28, 63	0
2	E	363/366 (99%)	1.54	104 (28%)	1 1	6, 20, 53, 78	0
All	All	1560/1568 (99%)	0.94	281 (18%)	2 2	6, 20, 42, 78	0

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	67	ILE	8.8
2	E	6	VAL	8.3
2	E	4	GLU	8.1
2	E	207	ILE	7.8
2	E	229	MET	7.5
1	A	417	TRP	7.4
1	D	1	SER	7.3
1	D	72	GLY	6.8
2	E	184	ALA	6.5
1	D	47	LEU	6.4
2	E	232	LYS	6.3
2	E	183	GLY	6.2
2	E	233	THR	6.1
2	E	234	ILE	5.9
2	E	210	THR	5.9
1	D	273	TRP	5.7
1	D	81	TYR	5.5
2	E	5	GLY	5.5
1	D	88	ILE	5.4
2	E	205	GLU	5.4
1	D	417	TRP	5.3

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Mol	Chain	Res	Type	RSRZ
2	E	209	LYS	5.3
2	E	185	VAL	5.2
2	E	186	HIS	5.2
2	E	7	LYS	5.2
1	D	43	GLY	5.1
2	E	202	PRO	5.0
1	D	229	ARG	5.0
2	E	188	SER	4.7
1	D	33	ALA	4.6
1	D	46	GLY	4.5
1	D	86	GLU	4.5
1	A	407	TYR	4.5
2	E	187	ALA	4.4
2	E	77	TYR	4.4
1	D	22	LYS	4.4
2	E	116	GLY	4.3
2	E	211	CYS	4.3
1	D	40	MET	4.3
1	D	207	MET	4.3
2	E	181	MET	4.3
1	A	250	LYS	4.3
1	A	415	GLY	4.3
1	D	132	SER	4.3
1	A	416	MET	4.2
1	D	276	LYS	4.2
1	A	411	LEU	4.2
1	D	106	PHE	4.2
1	A	406	ALA	4.1
1	D	45	ARG	4.1
1	D	24	THR	4.1
2	E	85	THR	4.1
2	E	132	VAL	4.1
1	D	228	ALA	4.0
2	E	182	CYS	4.0
1	D	38	VAL	4.0
2	E	27	TYR	4.0
1	D	89	PRO	4.0
2	E	230	LYS	4.0
2	E	92	PHE	3.9
2	E	201	ILE	3.9
2	E	200	PRO	3.9
1	D	131	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	332	GLU	3.9
2	E	86	SER	3.8
2	E	231	ASN	3.8
1	D	320	GLY	3.8
1	D	313	GLY	3.8
2	E	206	ALA	3.8
1	D	83	ASP	3.7
2	E	281	LEU	3.7
1	D	93	HIS	3.7
1	D	223	CYS	3.7
1	D	64	HIS	3.7
2	E	208	ARG	3.7
1	D	242	ILE	3.7
2	E	227	PRO	3.6
2	E	174	SER	3.6
2	E	82	LEU	3.6
2	E	213	ILE	3.6
1	D	94	PHE	3.5
2	B	187	ALA	3.5
2	E	254	MET	3.4
1	D	48	LEU	3.4
1	D	323	ILE	3.4
2	E	255	PRO	3.4
1	D	277	GLU	3.4
1	D	105	TRP	3.4
1	D	160	PHE	3.4
1	D	278	LEU	3.4
1	D	2	GLU	3.3
1	A	414	ARG	3.3
2	E	109	GLU	3.3
2	E	219	ALA	3.3
2	E	87	ARG	3.3
2	E	355	TYR	3.3
1	D	318	VAL	3.3
1	D	87	GLN	3.3
1	D	85	GLY	3.2
1	D	258	ILE	3.2
2	E	257	PHE	3.2
1	A	276	LYS	3.2
1	D	30	LYS	3.2
2	B	183	GLY	3.2
1	D	225	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	244	VAL	3.2
1	D	157	GLU	3.2
1	D	133	THR	3.2
1	D	115	LEU	3.1
2	E	52	TYR	3.1
1	D	130	HIS	3.1
1	A	413	LYS	3.1
2	E	204	ASP	3.1
2	B	5	GLY	3.1
1	D	84	LEU	3.1
1	D	150	PHE	3.1
2	E	26	ASN	3.0
2	E	252	PRO	3.0
1	D	5	LEU	3.0
1	D	92	GLU	3.0
1	D	31	ALA	3.0
2	E	84	TRP	3.0
1	D	62	TRP	3.0
2	E	248	TYR	3.0
2	E	73	ILE	3.0
1	D	256	MET	2.9
1	D	134	GLY	2.9
1	D	122	TRP	2.9
1	A	225	ALA	2.9
1	D	41	PRO	2.9
1	D	91	VAL	2.9
1	D	316	PRO	2.9
2	E	175	LEU	2.9
2	E	235	LYS	2.9
1	A	412	LYS	2.9
1	D	34	GLU	2.8
1	D	68	VAL	2.8
2	E	30	TRP	2.8
2	E	173	ILE	2.8
2	E	94	VAL	2.8
2	E	282	SER	2.8
2	E	110	ARG	2.8
1	D	18	VAL	2.8
1	D	280	ILE	2.8
2	E	32	TYR	2.8
1	D	25	ALA	2.8
1	D	49	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	151	GLU	2.8
2	E	203	ASN	2.8
1	A	323	ILE	2.7
1	D	42	LYS	2.7
2	B	184	ALA	2.7
2	E	134	THR	2.7
1	D	65	GLY	2.7
2	B	356	SER	2.7
2	E	253	GLY	2.7
2	B	272	LEU	2.7
1	D	199	TYR	2.7
2	E	238	VAL	2.7
1	D	272	LYS	2.7
1	D	71	VAL	2.7
2	E	103	LEU	2.6
2	E	256	LEU	2.6
1	D	255	TRP	2.6
2	E	133	HIS	2.6
1	A	255	TRP	2.6
1	D	249	VAL	2.6
2	E	65	TYR	2.6
2	E	236	VAL	2.6
1	D	59	LYS	2.6
1	D	227	LYS	2.6
1	D	148	PRO	2.6
2	E	56	PHE	2.6
1	D	53	ILE	2.6
1	D	66	GLY	2.5
2	E	298	THR	2.5
1	A	398	GLU	2.5
1	D	36	LYS	2.5
1	D	243	LYS	2.5
1	D	317	PHE	2.5
2	E	284	VAL	2.5
2	E	88	ASN	2.5
1	A	402	LEU	2.5
1	D	44	ALA	2.5
2	B	355	TYR	2.5
2	E	297	PRO	2.5
2	E	131	ILE	2.5
2	B	175	LEU	2.5
2	E	272	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	360	ALA	2.4
1	D	175	CYS	2.4
1	D	230	SER	2.4
1	D	321	ALA	2.4
2	B	281	LEU	2.4
2	E	353	TYR	2.4
2	E	98	SER	2.4
1	D	28	MET	2.4
1	A	224	VAL	2.4
1	D	178	PRO	2.4
2	B	186	HIS	2.4
1	A	408	THR	2.4
1	D	129	PHE	2.4
1	D	262	VAL	2.4
2	E	93	PHE	2.4
1	D	254	SER	2.4
1	D	162	ILE	2.4
2	B	185	VAL	2.4
1	D	314	LYS	2.4
2	E	100	ILE	2.4
2	E	366	TRP	2.4
2	E	214	PRO	2.3
2	B	181	MET	2.3
1	A	322	VAL	2.3
1	A	399	LYS	2.3
1	D	63	LYS	2.3
2	E	104	ILE	2.3
1	D	9	LEU	2.3
1	D	298	ALA	2.3
1	A	279	THR	2.3
1	D	279	THR	2.3
2	E	356	SER	2.3
1	D	304	GLU	2.3
2	E	280	GLU	2.3
1	D	333	VAL	2.3
1	D	37	ASP	2.3
2	E	130	ASN	2.3
1	D	21	ILE	2.3
2	E	216	THR	2.2
2	E	72	ASP	2.2
1	D	51	LEU	2.2
1	D	144	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	277	GLU	2.2
1	D	183	PHE	2.2
2	B	4	GLU	2.2
1	D	126	LEU	2.2
1	A	404	PRO	2.2
1	D	145	TYR	2.2
2	B	353	TYR	2.2
2	E	81	TYR	2.2
2	E	352	PRO	2.2
1	A	249	VAL	2.2
1	D	226	SER	2.2
1	D	259	GLU	2.2
2	E	212	GLU	2.2
2	E	228	ASP	2.2
2	E	140	CYS	2.2
2	B	351	THR	2.2
1	A	410	GLU	2.2
1	D	54	SER	2.2
1	D	224	VAL	2.2
2	E	354	PHE	2.2
2	E	288	TRP	2.2
2	E	129	SER	2.2
1	A	228	ALA	2.1
2	E	350	ILE	2.1
1	D	112	LEU	2.1
1	D	264	LYS	2.1
1	D	180	LEU	2.1
1	D	95	HIS	2.1
1	D	39	LYS	2.1
1	D	58	LYS	2.1
1	D	322	VAL	2.1
1	D	330	PHE	2.1
1	D	50	GLN	2.1
2	B	134	THR	2.1
1	D	271	ILE	2.1
1	D	246	GLN	2.1
1	D	303	ASP	2.1
1	D	247	GLU	2.1
1	D	23	LYS	2.1
2	B	132	VAL	2.1
2	E	270	GLY	2.1
2	E	239	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	142	ARG	2.0
1	D	282	ASN	2.0
1	A	247	GLU	2.0
1	A	405	SER	2.0
2	E	172	ARG	2.0
1	D	339	GLU	2.0
1	A	274	ASP	2.0
2	E	224	ALA	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	0.88	0.25	0.16	16,20,24,28	0
3	SRM	D	580	63/63	0.85	0.28	0.01	40,55,58,60	0
4	SF4	E	585	8/8	0.93	0.18	-0.67	70,74,77,78	0
3	SRM	A	580	63/63	0.95	0.15	-0.69	23,27,36,40	0
3	SRM	B	570	63/63	0.96	0.14	-0.94	13,16,20,23	0
4	SF4	D	575	8/8	0.93	0.13	-1.14	14,15,16,16	0
5	PO4	A	590	5/5	0.97	0.14	-1.25	59,59,61,63	0
4	SF4	E	586	8/8	0.96	0.12	-1.40	35,38,39,43	0
4	SF4	D	576	8/8	0.92	0.10	-1.49	17,20,21,22	0
4	SF4	A	575	8/8	0.98	0.10	-1.89	14,16,18,20	0
4	SF4	A	576	8/8	0.95	0.05	-2.64	13,14,15,16	0
4	SF4	B	586	8/8	0.98	0.06	-2.70	15,17,18,19	0
4	SF4	B	585	8/8	0.98	0.06	-2.74	21,24,28,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.