



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3MMA
Title : Dissimilatory sulfite reductase phosphate complex
Authors : Parey, K.; Warkentin, E.; Kroneck, P.M.H.; Ermler, U.
Deposited on : 2010-04-19
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

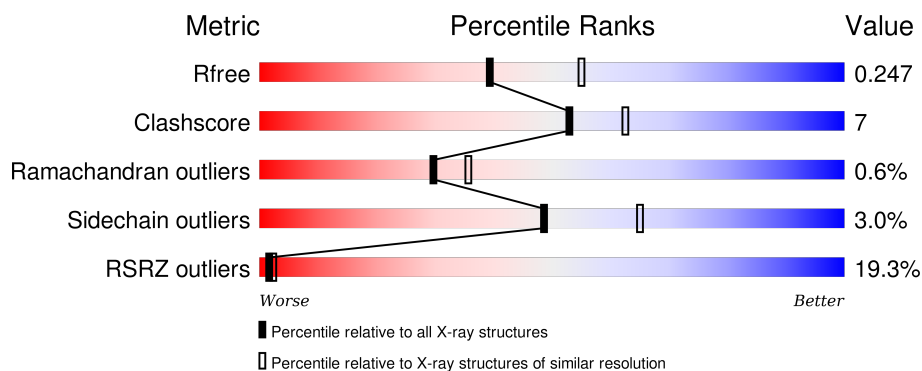
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 ≥ 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	
1	D	418	
2	B	366	
2	E	366	

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.

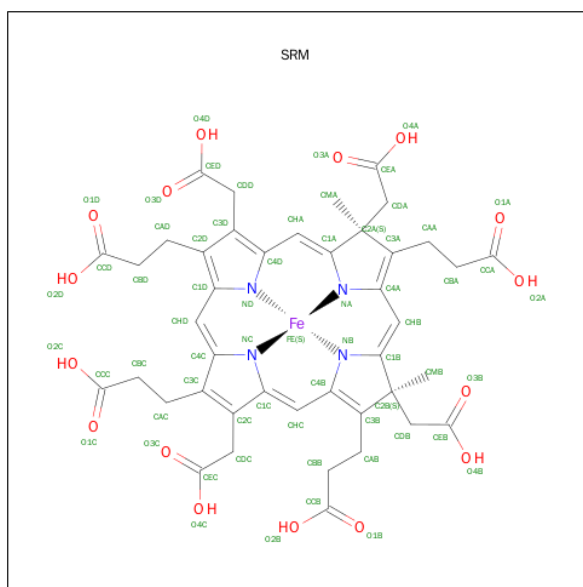
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

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.

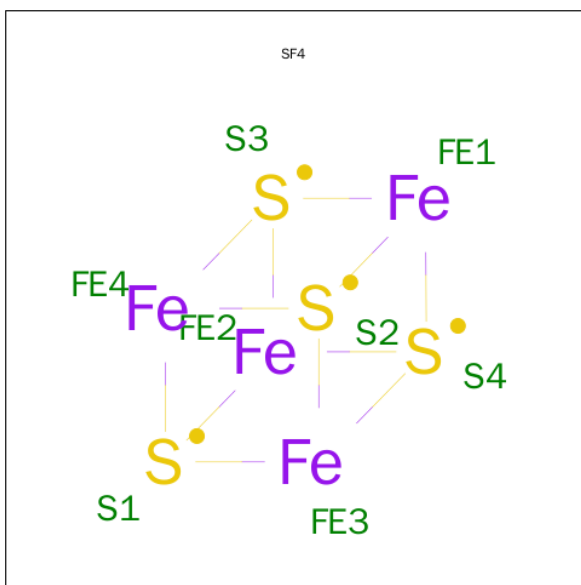
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			
2	E	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			

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



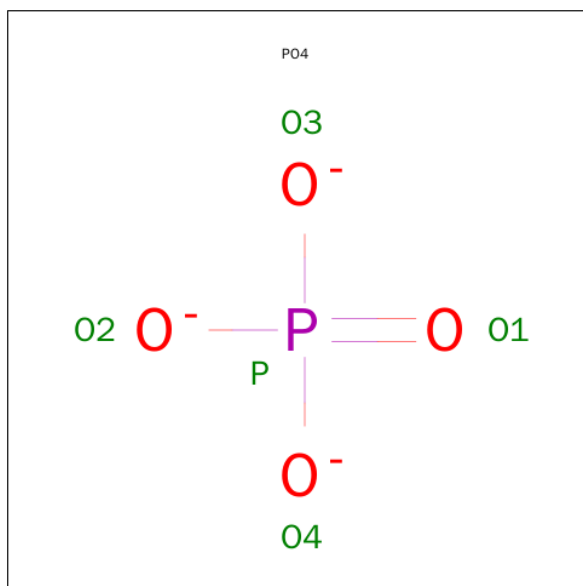
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	B	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	D	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	E	1	Total	C	Fe	N	O	
			63	42	1	4	16	

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



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

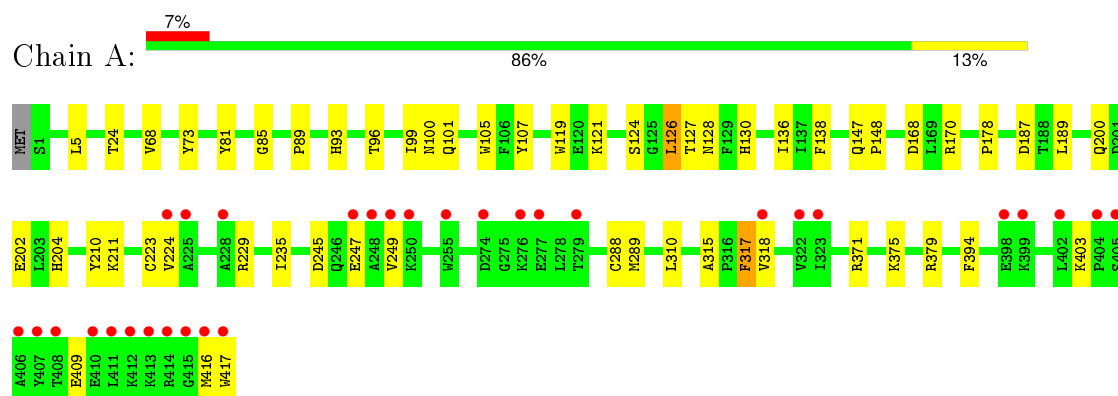
- Molecule 6 is water.

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		

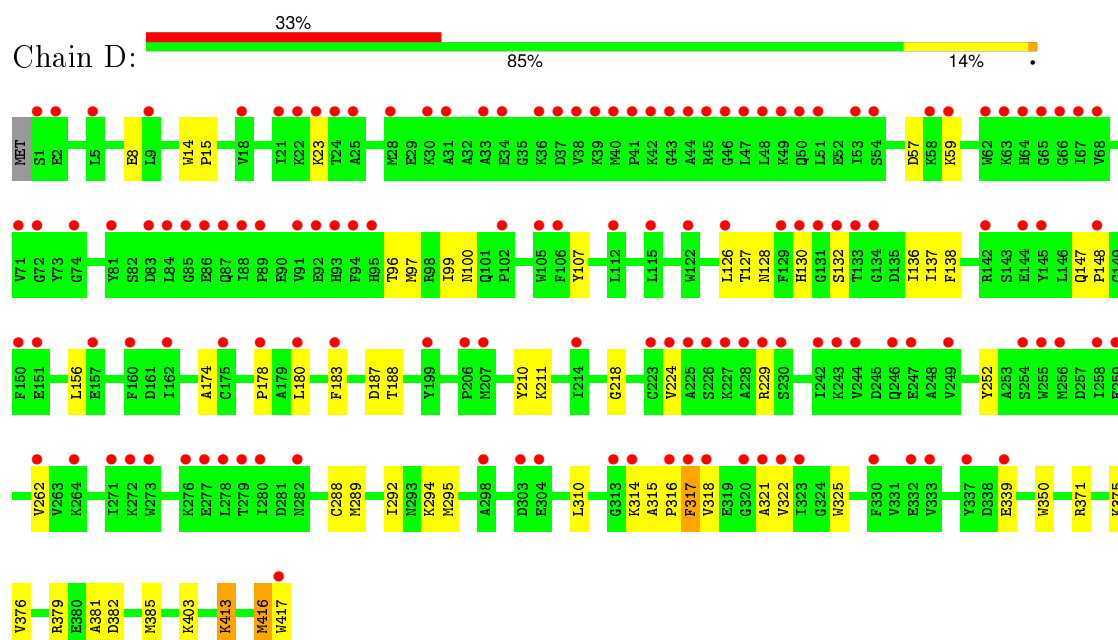
3 Residue-property plots

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.

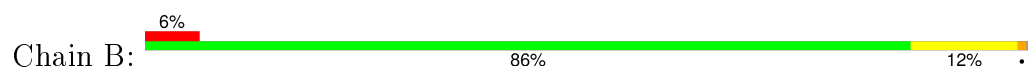
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

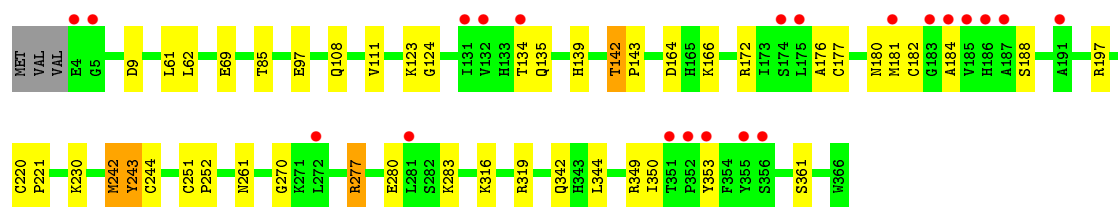


- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha



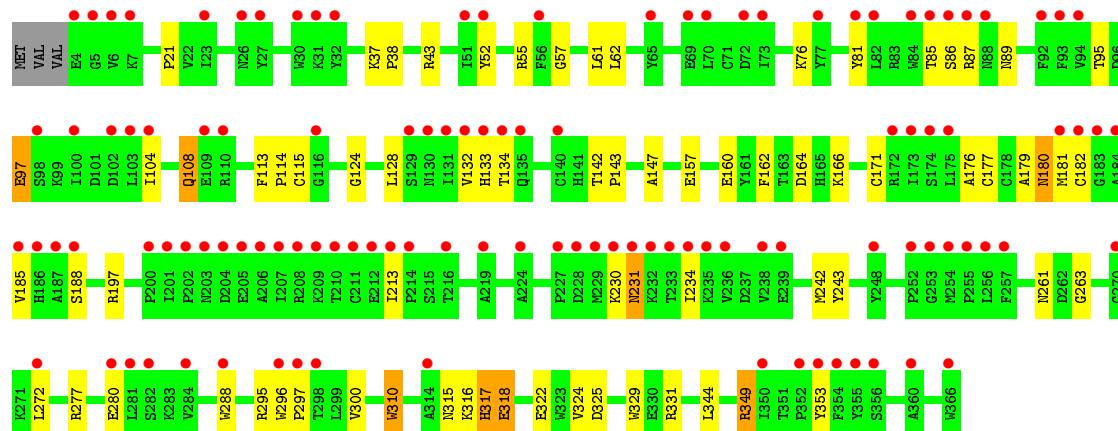
- Molecule 2: Sulfite reductase, dissimilatory-type subunit beta





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

Chain E: 31% 79% 18% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	34.8	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.2	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 78591 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12960	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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
3:E:570:SRM:HDD2	3:E:570:SRM:CBD	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:157:GLU:HG3	2:E:300:VAL:HG11	1.55	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
2:E:86:SER:OG	3:E:570:SRM:HAB1	1.96	0.65
1:D:379:ARG:HG3	1:D:379:ARG:HH11	1.61	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
2:E:272:LEU:HB2	3:E:570:SRM:CCC	2.33	0.59
2:B:350:ILE:O	2:E:349:ARG:NH2	2.28	0.59
1:A:394:PHE:HE2	2:E:179:ALA:HB1	1.68	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
2:E:37:LYS:HB2	2:E:38:PRO:CD	2.36	0.55
1:A:119:TRP:CH2	1:A:138:PHE:HB3	2.41	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
3:E:570:SRM:CBA	3:E:570:SRM:CHB	2.91	0.48
1:A:245:ASP:OD1	1:A:247:GLU:HG2	2.14	0.48
2:E:316:LYS:O	2:E:317:HIS:HB2	2.14	0.47
2:B:353:TYR:HA	2:E:353:TYR:HA	1.96	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:D:107:TYR:OH	1:D:130:HIS:CE1	2.67	0.45
1:A:200:GLN:NE2	1:A:204:HIS:NE2	2.65	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:D:316:PRO:HA	1:D:321:ALA:N	2.32	0.44
1:A:127:THR:O	2:B:61:LEU:HD12	2.17	0.44
3:B:570:SRM:HDD2	3:B:570:SRM:HBD2	1.99	0.44
2:B:242:MET:SD	2:B:244:CYS:HB3	2.58	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
3:A:580:SRM:HMB3	3:A:580:SRM:HBB2	2.00	0.43
1:A:379:ARG:NH1	1:A:379:ARG:CG	2.81	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
1:D:127:THR:O	2:E:61:LEU:HD12	2.20	0.42
2:B:342:GLN:HB3	1:D:381:ALA:HB2	2.02	0.42
2:E:296:TRP:N	2:E:297:PRO:HD3	2.34	0.42
2:B:164:ASP:HB3	2:B:166:LYS:HG3	2.01	0.42
3:A:580:SRM:CMB	3:A:580:SRM:HBB2	2.48	0.42
1:D:132:SER:H	3:D:580:SRM:HBB1	1.83	0.42
2:B:188:SER:N	2:B:270:GLY:HA3	2.35	0.42
1:A:85:GLY:O	1:A:89:PRO:HA	2.20	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:D:315:ALA:HB3	3:D:580:SRM:HBD1	2.01	0.41
1:A:73:TYR:CD1	1:A:204:HIS:HB3	2.55	0.41
2:B:251:CYS:HA	2:B:252:PRO:HD2	1.88	0.41
2:B:123:LYS:HA	2:B:123:LYS:HD2	1.92	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:HAC2	3:E:570:SRM:HCD1	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:277:ARG:NH2	2:E:280:GLU:OE1	2.50	0.40
2:E:213:ILE:HG23	2:E:234:ILE:HG12	2.03	0.40
2:B:319:ARG:HH22	3:B:570:SRM:CCC	2.34	0.40
1:A:178:PRO:HG3	1:A:187:ASP:HA	2.02	0.40
2:E:197:ARG:NH2	2:E:261:ASN:HD22	2.09	0.40
3:A:580:SRM:HAD1	3:A:580:SRM:O4D	2.22	0.40
1:A:119:TRP:CZ3	1:A:138:PHE:HB3	2.56	0.40
2:B:342:GLN:CD	1:D:371:ARG:HG3	2.42	0.40
1:A:81:TYR:CE2	1:A:93:HIS:CD2	3.10	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%)	52	64
1	D	415/418 (99%)	393 (95%)	21 (5%)	1 (0%)	52	64
2	B	361/366 (99%)	343 (95%)	16 (4%)	2 (1%)	30	36
2	E	361/366 (99%)	331 (92%)	25 (7%)	5 (1%)	14	13
All	All	1552/1568 (99%)	1469 (95%)	74 (5%)	9 (1%)	30	36

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%)	58	75
1	D	353/354 (100%)	344 (98%)	9 (2%)	55	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	314/317 (99%)	304 (97%)	10 (3%)	46	62
2	E	314/317 (99%)	301 (96%)	13 (4%)	37	50
All	All	1334/1342 (99%)	1294 (97%)	40 (3%)	48	65

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	29,70,70	2.05	6 (20%)	29,112,112	4.12	17 (58%)
5	PO4	A	590	-	4,4,4	0.70	0	6,6,6	0.29	0
3	SRM	B	570	1	29,70,70	2.63	9 (31%)	29,112,112	4.44	17 (58%)
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	2.10	8 (27%)	29,112,112	4.09	10 (34%)
3	SRM	E	570	-	29,70,70	2.86	10 (34%)	29,112,112	5.12	18 (62%)
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 (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	570	SRM	C4C-NC	-6.13	1.28	1.36
3	E	570	SRM	C1B-NB	-5.98	1.29	1.38
3	B	570	SRM	C4A-NA	-5.87	1.28	1.39
3	E	570	SRM	C1C-NC	-5.80	1.28	1.36
3	E	570	SRM	C4A-NA	-5.70	1.28	1.39
3	B	570	SRM	C4C-NC	-5.24	1.29	1.36
3	B	570	SRM	C1B-NB	-5.13	1.30	1.38
3	B	570	SRM	C1C-NC	-4.13	1.31	1.36
3	D	580	SRM	C4A-NA	-3.08	1.33	1.39
3	A	580	SRM	C4A-NA	-3.06	1.33	1.39
3	E	570	SRM	C4B-NB	-2.67	1.34	1.39
3	B	570	SRM	CDA-C2A	-2.62	1.52	1.56
3	D	580	SRM	C1A-NA	-2.60	1.34	1.38
3	A	580	SRM	C4C-NC	-2.33	1.33	1.36
3	E	570	SRM	C1A-NA	-2.33	1.34	1.38
3	E	570	SRM	CHC-C4B	-2.24	1.34	1.39
3	B	570	SRM	C1A-NA	-2.23	1.34	1.38
3	D	580	SRM	C4C-NC	-2.15	1.33	1.36
3	D	580	SRM	C4B-NB	-2.11	1.35	1.39
3	E	570	SRM	CHB-C4A	-2.07	1.34	1.39
3	B	570	SRM	CAA-C3A	2.94	1.56	1.51
3	D	580	SRM	FE-NA	3.49	2.09	1.95
3	D	580	SRM	FE-NB	3.53	2.09	1.95
3	A	580	SRM	FE-NB	3.60	2.10	1.95
3	A	580	SRM	C3C-C2C	3.84	1.49	1.37
3	A	580	SRM	FE-NA	4.08	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	5.76	1.52	1.39
3	E	570	SRM	C3D-C2D	6.13	1.53	1.39
3	A	580	SRM	C3D-C2D	6.59	1.54	1.39
3	D	580	SRM	C3D-C2D	6.68	1.54	1.39

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	580	SRM	CAB-C3B-C2B	-15.27	106.27	123.46
3	E	570	SRM	CAD-C2D-C1D	-13.02	112.87	127.01
3	B	570	SRM	CAA-C3A-C2A	-12.23	109.69	123.46
3	D	580	SRM	CAB-C3B-C2B	-11.93	110.02	123.46
3	D	580	SRM	CAD-C2D-C1D	-11.44	114.58	127.01
3	E	570	SRM	CAC-C3C-C4C	-10.78	115.30	127.01
3	E	570	SRM	CAA-C3A-C2A	-10.70	111.41	123.46
3	E	570	SRM	CDC-C2C-C1C	-8.96	112.92	127.38
3	E	570	SRM	C4A-NA-C1A	-8.21	102.44	106.90
3	A	580	SRM	CAD-C2D-C3D	-7.78	110.02	129.38
3	B	570	SRM	CEC-CDC-C2C	-6.91	103.11	116.31
3	B	570	SRM	C4A-NA-C1A	-6.74	103.24	106.90
3	B	570	SRM	CBC-CAC-C3C	-6.28	101.28	112.53
3	A	580	SRM	CAA-C3A-C2A	-5.41	117.38	123.46
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	D	580	SRM	CAA-C3A-C2A	-5.12	117.69	123.46
3	E	570	SRM	CAD-C2D-C3D	-4.61	117.90	129.38
3	B	570	SRM	CAC-C3C-C2C	-4.38	118.48	129.38
3	B	570	SRM	CAC-C3C-C4C	-4.30	122.34	127.01
3	E	570	SRM	CHB-C4A-C3A	-4.17	116.01	125.48
3	D	580	SRM	C4B-NB-C1B	-4.11	104.67	106.90
3	D	580	SRM	CDD-C3D-C4D	-3.95	120.92	127.34
3	B	570	SRM	CMA-C2A-CDA	-3.66	105.41	109.76
3	B	570	SRM	CHB-C4A-C3A	-3.58	117.35	125.48
3	E	570	SRM	CDD-C3D-C4D	-3.46	121.73	127.34
3	A	580	SRM	CAC-CBC-CCC	-3.32	106.66	112.75
3	E	570	SRM	CEC-CDC-C2C	-3.26	110.08	116.31
3	B	570	SRM	CDC-C2C-C1C	-3.14	122.31	127.38
3	A	580	SRM	C4B-NB-C1B	-3.08	105.23	106.90
3	A	580	SRM	CDD-C3D-C4D	-2.99	122.48	127.34
3	A	580	SRM	CAD-C2D-C1D	-2.94	123.82	127.01
3	B	570	SRM	CAB-C3B-C2B	-2.65	120.48	123.46
3	B	570	SRM	CAD-C2D-C3D	-2.63	122.83	129.38
3	A	580	SRM	CAD-CBD-CCD	-2.44	108.28	112.75
3	A	580	SRM	C3A-C4A-NA	-2.26	107.57	110.09
3	E	570	SRM	CBC-CAC-C3C	-2.17	108.63	112.53
3	E	570	SRM	C4B-NB-C1B	-2.16	105.73	106.90
3	E	570	SRM	CMA-C2A-CDA	-2.07	107.30	109.76
3	D	580	SRM	CAC-C3C-C4C	2.09	129.28	127.01
3	E	570	SRM	C2B-CDB-CEB	2.18	118.83	115.45
3	A	580	SRM	CBC-CAC-C3C	2.26	116.57	112.53
3	E	570	SRM	CAB-C3B-C2B	2.40	126.17	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	580	SRM	C3B-C4B-NB	2.49	112.86	110.09
3	A	580	SRM	CED-CDD-C3D	2.55	121.19	116.31
3	E	570	SRM	CED-CDD-C3D	2.57	121.22	116.31
3	E	570	SRM	CMB-C2B-CDB	2.66	112.93	109.76
3	A	580	SRM	C2A-CDA-CEA	2.81	119.81	115.45
3	B	570	SRM	CED-CDD-C3D	2.87	121.81	116.31
3	A	580	SRM	CDC-C2C-C1C	2.93	132.11	127.38
3	D	580	SRM	C3B-C4B-NB	3.37	113.83	110.09
3	B	570	SRM	CAA-CBA-CCA	3.70	119.52	112.75
3	A	580	SRM	CBD-CAD-C2D	4.02	119.74	112.53
3	A	580	SRM	CMA-C2A-CDA	4.89	115.59	109.76
3	B	570	SRM	C2B-CDB-CEB	5.09	123.34	115.45
3	B	570	SRM	CAB-CBB-CCB	5.34	122.53	112.75
3	D	580	SRM	CMA-C2A-CDA	5.89	116.78	109.76
3	A	580	SRM	C4A-NA-C1A	6.05	110.19	106.90
3	B	570	SRM	CBD-CAD-C2D	6.72	124.57	112.53
3	D	580	SRM	C4A-NA-C1A	7.41	110.92	106.90
3	B	570	SRM	C3A-C4A-NA	7.43	118.35	110.09
3	E	570	SRM	C3A-C4A-NA	8.58	119.62	110.09

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
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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	417/418 (99%)	0.45	31 (7%) 17 25	12, 19, 35, 78	0
1	D	417/418 (99%)	1.58	136 (32%) 1 0	13, 23, 36, 54	0
2	B	363/366 (99%)	0.41	21 (5%) 26 35	11, 18, 28, 63	0
2	E	363/366 (99%)	1.64	113 (31%) 1 1	6, 20, 53, 78	0
All	All	1560/1568 (99%)	1.02	301 (19%) 2 2	6, 20, 42, 78	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	67	ILE	9.1
2	E	6	VAL	8.7
2	E	4	GLU	8.3
2	E	207	ILE	8.1
2	E	229	MET	7.7
1	A	417	TRP	7.6
1	D	1	SER	7.6
1	D	72	GLY	7.0
2	E	184	ALA	6.7
1	D	47	LEU	6.6
2	E	183	GLY	6.4
2	E	232	LYS	6.4
2	E	233	THR	6.3
2	E	234	ILE	6.2
2	E	210	THR	6.2
1	D	273	TRP	5.9
2	E	5	GLY	5.7
1	D	81	TYR	5.7
1	D	88	ILE	5.6
2	E	205	GLU	5.5
1	D	417	TRP	5.5

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Mol	Chain	Res	Type	RSRZ
2	E	185	VAL	5.4
2	E	209	LYS	5.4
2	E	186	HIS	5.4
2	E	7	LYS	5.3
1	D	43	GLY	5.3
2	E	202	PRO	5.2
1	D	229	ARG	5.1
2	E	188	SER	4.9
1	D	33	ALA	4.7
1	D	46	GLY	4.7
1	D	86	GLU	4.6
2	E	187	ALA	4.6
1	A	407	TYR	4.6
2	E	211	CYS	4.5
2	E	77	TYR	4.5
2	E	116	GLY	4.5
1	D	22	LYS	4.5
1	D	40	MET	4.4
1	D	207	MET	4.4
1	A	415	GLY	4.4
1	D	132	SER	4.4
2	E	181	MET	4.4
1	A	416	MET	4.4
1	A	250	LYS	4.4
1	A	411	LEU	4.3
1	D	106	PHE	4.3
1	D	276	LYS	4.3
1	A	406	ALA	4.3
2	E	132	VAL	4.3
1	D	24	THR	4.3
2	E	85	THR	4.3
2	E	182	CYS	4.2
1	D	38	VAL	4.2
1	D	45	ARG	4.2
1	D	228	ALA	4.2
1	D	89	PRO	4.1
2	E	27	TYR	4.1
2	E	201	ILE	4.1
2	E	230	LYS	4.1
2	E	92	PHE	4.1
2	E	200	PRO	4.1
1	D	131	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	332	GLU	4.0
2	E	86	SER	4.0
2	E	231	ASN	3.9
1	D	320	GLY	3.9
2	E	206	ALA	3.9
1	D	313	GLY	3.9
1	D	223	CYS	3.9
2	E	281	LEU	3.9
1	D	83	ASP	3.9
1	D	93	HIS	3.9
1	D	64	HIS	3.8
1	D	242	ILE	3.8
2	E	227	PRO	3.8
2	E	174	SER	3.8
2	E	208	ARG	3.8
2	E	82	LEU	3.7
2	E	213	ILE	3.7
2	B	187	ALA	3.6
1	D	94	PHE	3.6
1	D	323	ILE	3.6
1	D	48	LEU	3.6
2	E	254	MET	3.6
2	E	255	PRO	3.6
1	D	105	TRP	3.6
1	D	277	GLU	3.5
1	D	278	LEU	3.5
1	D	160	PHE	3.5
1	D	318	VAL	3.4
1	D	2	GLU	3.4
2	E	219	ALA	3.4
2	E	109	GLU	3.4
1	A	414	ARG	3.4
1	D	258	ILE	3.4
2	E	355	TYR	3.4
1	D	85	GLY	3.4
2	E	257	PHE	3.4
2	E	87	ARG	3.4
1	D	87	GLN	3.4
1	D	225	ALA	3.4
2	B	183	GLY	3.4
1	D	244	VAL	3.3
1	A	276	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	133	THR	3.3
1	D	30	LYS	3.3
1	D	157	GLU	3.3
1	D	115	LEU	3.3
1	D	130	HIS	3.2
2	B	5	GLY	3.2
2	E	204	ASP	3.2
2	E	52	TYR	3.2
1	D	84	LEU	3.2
1	D	150	PHE	3.2
1	A	413	LYS	3.2
2	E	252	PRO	3.2
2	E	26	ASN	3.2
1	D	31	ALA	3.1
1	D	5	LEU	3.1
2	E	84	TRP	3.1
1	D	62	TRP	3.1
2	E	73	ILE	3.1
1	D	92	GLU	3.1
2	E	248	TYR	3.1
1	D	134	GLY	3.1
1	D	256	MET	3.1
1	D	91	VAL	3.1
1	D	122	TRP	3.1
1	A	225	ALA	3.0
1	D	41	PRO	3.0
1	D	316	PRO	3.0
2	E	175	LEU	3.0
1	D	68	VAL	3.0
2	E	94	VAL	3.0
2	E	173	ILE	3.0
2	E	30	TRP	3.0
1	D	18	VAL	3.0
2	E	235	LYS	2.9
1	D	34	GLU	2.9
1	A	412	LYS	2.9
1	D	280	ILE	2.9
2	E	282	SER	2.9
1	D	25	ALA	2.9
2	E	32	TYR	2.9
2	E	110	ARG	2.9
1	A	323	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	203	ASN	2.9
2	B	184	ALA	2.9
2	E	134	THR	2.9
1	D	151	GLU	2.9
1	D	49	LYS	2.9
1	D	65	GLY	2.8
2	B	356	SER	2.8
2	E	253	GLY	2.8
2	E	238	VAL	2.8
2	B	272	LEU	2.8
1	D	42	LYS	2.8
1	D	71	VAL	2.8
1	D	199	TYR	2.8
2	E	103	LEU	2.8
2	E	256	LEU	2.8
1	D	255	TRP	2.8
1	D	249	VAL	2.7
2	E	236	VAL	2.7
2	E	133	HIS	2.7
1	D	272	LYS	2.7
1	A	255	TRP	2.7
2	E	65	TYR	2.7
1	D	53	ILE	2.7
1	D	148	PRO	2.7
2	E	56	PHE	2.7
1	D	66	GLY	2.7
2	E	298	THR	2.7
1	D	59	LYS	2.7
1	D	227	LYS	2.7
2	E	284	VAL	2.6
1	D	317	PHE	2.6
1	D	175	CYS	2.6
1	A	402	LEU	2.6
1	D	44	ALA	2.6
2	E	131	ILE	2.6
1	A	398	GLU	2.6
2	E	88	ASN	2.6
2	E	297	PRO	2.6
2	B	175	LEU	2.6
2	E	272	LEU	2.6
2	E	360	ALA	2.6
1	D	36	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	243	LYS	2.6
2	B	355	TYR	2.6
1	D	321	ALA	2.6
1	D	230	SER	2.5
1	A	224	VAL	2.5
1	D	262	VAL	2.5
2	B	281	LEU	2.5
1	A	408	THR	2.5
2	B	185	VAL	2.5
1	D	162	ILE	2.5
2	E	98	SER	2.5
1	D	129	PHE	2.5
1	D	178	PRO	2.5
2	B	186	HIS	2.5
2	E	93	PHE	2.5
2	E	353	TYR	2.5
1	D	28	MET	2.5
1	D	254	SER	2.5
2	E	100	ILE	2.5
2	E	366	TRP	2.5
2	E	214	PRO	2.5
1	A	322	VAL	2.5
2	B	181	MET	2.4
2	E	104	ILE	2.4
1	D	314	LYS	2.4
1	D	298	ALA	2.4
1	A	279	THR	2.4
1	D	279	THR	2.4
1	D	9	LEU	2.4
2	E	356	SER	2.4
1	D	333	VAL	2.4
1	A	399	LYS	2.4
1	D	21	ILE	2.4
1	D	63	LYS	2.4
1	D	304	GLU	2.4
2	E	216	THR	2.4
1	D	37	ASP	2.4
2	E	130	ASN	2.4
2	E	280	GLU	2.4
2	E	72	ASP	2.3
1	D	51	LEU	2.3
2	E	140	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	249	VAL	2.3
1	D	183	PHE	2.3
1	D	126	LEU	2.3
1	D	144	GLU	2.3
1	D	224	VAL	2.3
1	A	404	PRO	2.3
2	E	352	PRO	2.3
2	B	351	THR	2.3
1	A	277	GLU	2.3
1	D	226	SER	2.3
2	E	228	ASP	2.3
1	D	145	TYR	2.3
2	B	353	TYR	2.3
2	E	81	TYR	2.3
2	B	4	GLU	2.3
2	E	354	PHE	2.3
1	D	54	SER	2.3
2	E	288	TRP	2.3
1	D	259	GLU	2.3
2	E	212	GLU	2.3
2	E	350	ILE	2.3
1	A	228	ALA	2.3
2	E	129	SER	2.3
1	A	410	GLU	2.3
1	D	112	LEU	2.3
1	D	322	VAL	2.2
1	D	180	LEU	2.2
1	D	95	HIS	2.2
1	D	330	PHE	2.2
2	B	134	THR	2.2
1	D	271	ILE	2.2
1	D	264	LYS	2.2
2	B	132	VAL	2.2
1	D	303	ASP	2.2
1	D	39	LYS	2.2
1	D	50	GLN	2.2
1	D	58	LYS	2.2
2	E	270	GLY	2.2
1	D	246	GLN	2.2
1	D	247	GLU	2.2
1	D	282	ASN	2.1
1	A	405	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	239	GLU	2.1
1	D	23	LYS	2.1
1	D	142	ARG	2.1
1	A	247	GLU	2.1
2	E	224	ALA	2.1
2	E	23	ILE	2.1
1	D	206	PRO	2.1
1	A	274	ASP	2.1
2	E	172	ARG	2.1
1	D	74	GLY	2.1
1	D	102	PRO	2.1
1	D	339	GLU	2.1
2	E	296	TRP	2.1
1	D	214	ILE	2.1
2	E	102	ASP	2.1
1	D	337	TYR	2.1
1	A	248	ALA	2.1
2	B	174	SER	2.1
2	E	31	LYS	2.1
2	E	69	GLU	2.0
2	E	70	LEU	2.0
2	E	314	ALA	2.0
2	B	131	ILE	2.0
2	E	51	ILE	2.0
2	E	135	GLN	2.0
2	B	352	PRO	2.0
1	A	318	VAL	2.0
2	B	191	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SRM	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

There are no such residues in this entry.