



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:07 pm BST

PDB ID : 2XWZ
Title : STRUCTURE OF THE RECOMBINANT NATIVE NITRITE REDUCTASE
FROM *ALCALIGENES XYLOSOXIDANS* complexed with nitrite
Authors : Antonyuk, S.V.; Leferink, N.G.H.; Han, C.; Heyes, D.J.; Rigby, S.E.J.; Hough,
M.A.; Eady, R.R.; Scrutton, N.S.; Hasnain, S.S.
Deposited on : 2010-11-06
Resolution : 2.34 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

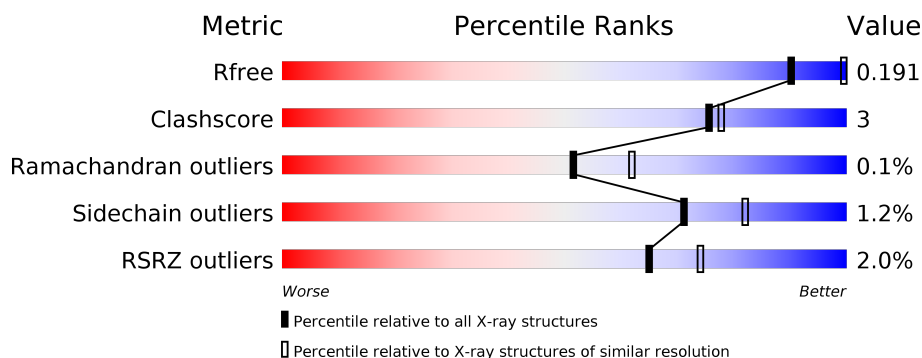
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 respectively. 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	336	<div> <div>2%</div> <div>92%</div> <div>8%</div> </div>
1	B	336	<div> <div>2%</div> <div>93%</div> <div>7%</div> </div>
1	C	336	<div> <div>2%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	D	336	<div> <div>%</div> <div>91%</div> <div>9%</div> </div>
1	E	336	<div> <div>3%</div> <div>95%</div> <div>.</div> </div>
1	F	336	<div> <div>2%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	F	1342	-	-	X	-
5	ACT	B	1343	-	-	X	-
5	ACT	C	1337	-	-	X	-
5	ACT	D	1338	-	-	X	-
5	ACT	E	1338	-	-	X	-
5	ACT	E	1339	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17342 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 DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	3	0
			2587	1647	450	479	11			
1	B	335	Total	C	N	O	S	0	1	0
			2569	1635	446	477	11			
1	C	335	Total	C	N	O	S	0	2	0
			2576	1640	447	478	11			
1	D	335	Total	C	N	O	S	0	3	0
			2582	1644	448	479	11			
1	E	335	Total	C	N	O	S	0	2	0
			2574	1638	446	479	11			
1	F	334	Total	C	N	O	S	0	5	0
			2586	1648	447	480	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	expression tag	UNP O68601
B	1	GLU	-	expression tag	UNP O68601
C	1	GLU	-	expression tag	UNP O68601
D	1	GLU	-	expression tag	UNP O68601
E	1	GLU	-	expression tag	UNP O68601
F	1	GLU	-	expression tag	UNP O68601

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

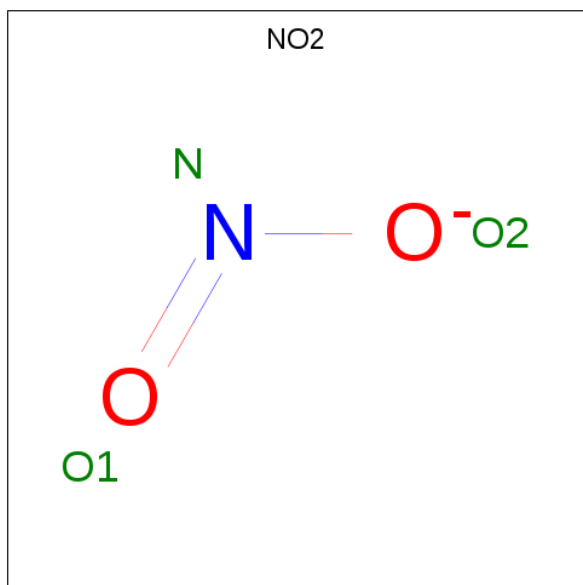
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Cu	0	0
			2	2		
2	E	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total	Cu	0	0
			2	2		
2	A	2	Total	Cu	0	0
			2	2		
2	F	2	Total	Cu	0	0
			2	2		

- Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			3	1	2		
3	A	1	Total	N	O	0	0
			3	1	2		
3	B	1	Total	N	O	0	0
			3	1	2		
3	F	1	Total	N	O	0	0
			3	1	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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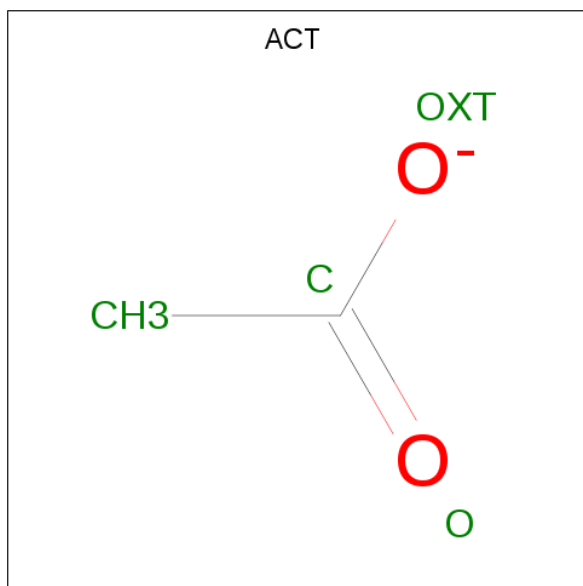
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	1
			10	8	2		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



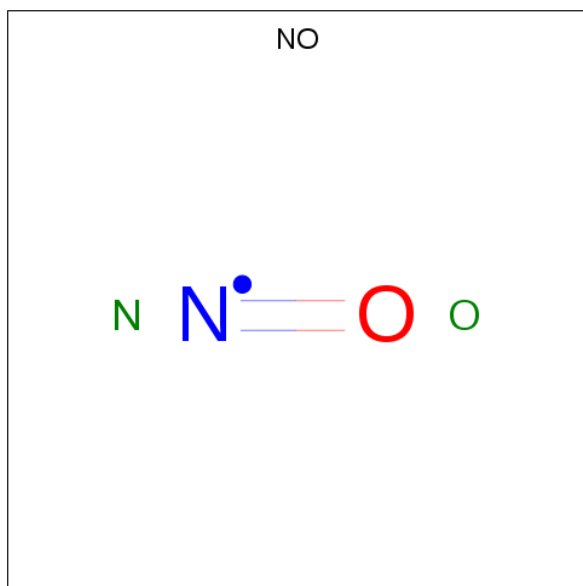
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is NITRIC OXIDE (three-letter code: NO) (formula: NO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	N	O	0	0
			2	1	1		
6	E	1	Total	N	O	0	0
			2	1	1		

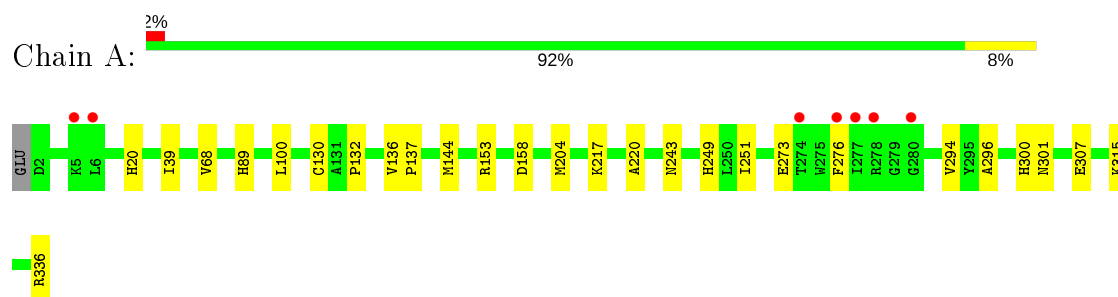
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	275	Total 275	O 275	0	0
7	B	234	Total 234	O 234	0	0
7	C	258	Total 258	O 258	0	0
7	D	261	Total 261	O 261	0	0
7	E	277	Total 277	O 277	0	0
7	F	266	Total 266	O 266	0	0

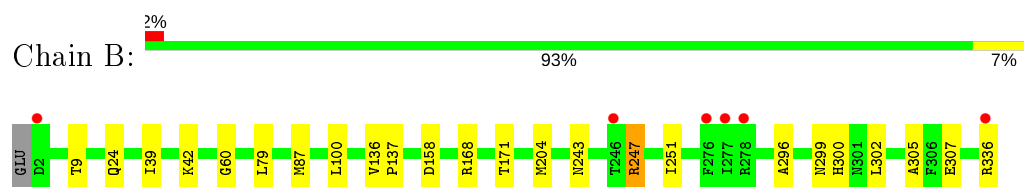
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

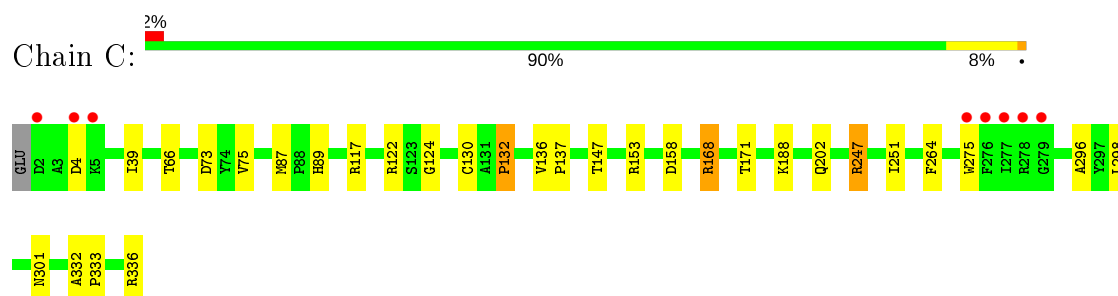
• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE



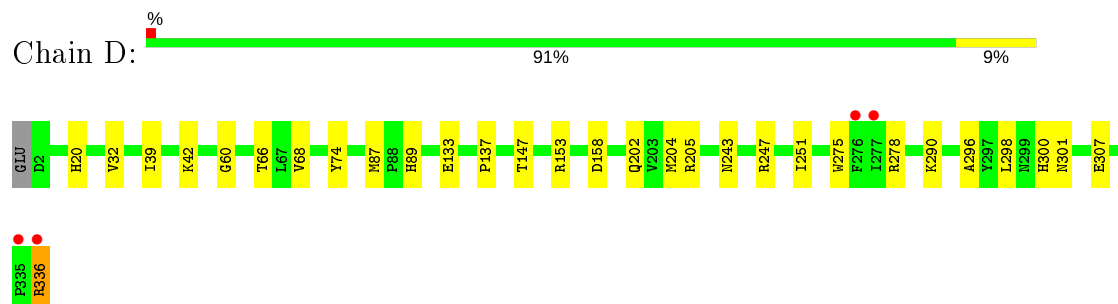
• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE



• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

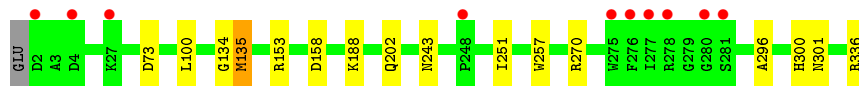


• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

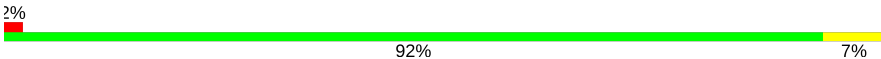


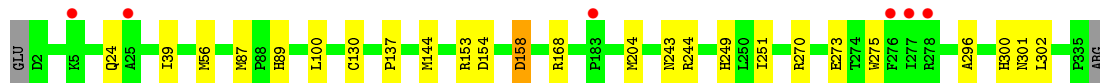
● Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain E: 



● Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.93Å 176.82Å 181.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.97 – 2.34 43.97 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.97-2.34) 99.4 (43.97-2.34)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.174 , 0.199 0.168 , 0.191	Depositor DCC
R_{free} test set	11648 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k 0.004 for -l,-k,-h 0.007 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17342	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: SO4, ACT, NO2, CU, NO

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	0.75	0/2667	0.78	3/3629 (0.1%)
1	B	0.73	0/2643	0.77	2/3599 (0.1%)
1	C	0.78	0/2653	0.78	1/3612 (0.0%)
1	D	0.77	0/2662	0.78	1/3624 (0.0%)
1	E	0.78	0/2651	0.76	1/3610 (0.0%)
1	F	0.76	1/2672 (0.0%)	0.77	2/3638 (0.1%)
All	All	0.76	1/15948 (0.0%)	0.78	10/21712 (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
1	B	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	130	CYS	CB-SG	-5.56	1.72	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ARG	NE-CZ-NH2	-6.26	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ARG	CG-CD-NE	-5.83	99.56	111.80
1	A	144	MET	CG-SD-CE	-5.78	90.96	100.20
1	B	158	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	247	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	F	244	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	E	135	MET	CG-SD-CE	5.12	108.39	100.20
1	D	153	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	F	153	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	122	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	HIS	Peptide
1	B	300	HIS	Peptide
1	D	300	HIS	Peptide
1	E	300	HIS	Peptide
1	F	300	HIS	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	2587	0	2555	15	0
1	B	2569	0	2525	16	0
1	C	2576	0	2535	21	0
1	D	2582	0	2539	23	0
1	E	2574	0	2529	10	0
1	F	2586	0	2554	17	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	F	3	0	0	0	0
4	A	35	0	0	0	0
4	B	40	0	0	2	0
4	C	30	0	0	0	0
4	D	50	0	0	1	0
4	E	35	0	0	0	0
4	F	35	0	0	2	0
5	A	4	0	3	0	0
5	B	12	0	9	4	0
5	C	4	0	3	4	0
5	D	8	0	6	2	0
5	E	12	0	9	6	0
5	F	4	0	3	0	0
6	C	2	0	0	0	0
6	E	2	0	0	0	0
7	A	275	0	0	0	0
7	B	234	0	0	6	0
7	C	258	0	0	3	0
7	D	261	0	0	3	0
7	E	277	0	0	2	0
7	F	266	0	0	1	0
All	All	17342	0	15270	95	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 3.

All (95) 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)
1:B:87:MET:HE2	7:B:2096:HOH:O	1.59	1.01
1:A:307:GLU:OE2	5:D:1338:ACT:H1	1.68	0.93
1:D:87:MET:HE2	7:D:2116:HOH:O	1.75	0.85
1:B:87:MET:CE	7:B:2096:HOH:O	2.17	0.84
1:D:290:LYS:NZ	5:E:1339:ACT:H1	1.96	0.81
1:D:202[B]:GLN:OE1	1:D:205[B]:ARG:NH1	2.15	0.80
1:B:251:ILE:HD12	1:B:296:ALA:HB3	1.69	0.74
4:B:1345:SO4:O1	7:B:2229:HOH:O	2.07	0.72
1:C:202[B]:GLN:OE1	7:C:2168:HOH:O	2.08	0.71
4:B:1347:SO4:O4	7:B:2230:HOH:O	2.07	0.70
1:B:307:GLU:OE2	5:C:1337:ACT:H3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:HD11	1:B:79:LEU:HD11	1.75	0.68
1:D:290:LYS:HZ1	5:E:1339:ACT:H1	1.56	0.68
1:E:188:LYS:HD2	7:E:2172:HOH:O	1.95	0.66
1:E:251:ILE:HD12	1:E:296:ALA:HB3	1.78	0.65
1:B:307:GLU:OE2	5:C:1337:ACT:CH3	2.44	0.65
4:D:1348:SO4:O3	7:D:2260:HOH:O	2.12	0.65
1:C:188:LYS:HD2	7:C:2166:HOH:O	1.98	0.63
1:B:137:PRO:HB2	1:B:204:MET:HE1	1.80	0.63
1:A:20:HIS:CE1	1:A:68:VAL:H	2.18	0.62
5:B:1343:ACT:H1	1:F:270:ARG:NH2	2.15	0.61
1:F:154[B]:ASP:HB2	4:F:1342:SO4:O2	2.01	0.61
1:D:137:PRO:HG2	5:D:1338:ACT:H2	1.81	0.61
1:D:137:PRO:HB2	1:D:204:MET:HE1	1.84	0.60
1:D:290:LYS:HZ3	5:E:1339:ACT:H1	1.69	0.57
1:A:100:LEU:HA	1:E:251:ILE:HG22	1.87	0.56
1:C:168:ARG:NH2	7:C:2131:HOH:O	2.40	0.54
1:D:251:ILE:HD12	1:D:296:ALA:HB3	1.89	0.54
1:A:20:HIS:HE1	1:A:68:VAL:H	1.56	0.53
5:B:1343:ACT:H2	7:B:2058:HOH:O	2.09	0.53
1:C:87:MET:HA	1:C:87:MET:HE3	1.91	0.53
1:D:39:ILE:HD13	1:D:89:HIS:HB2	1.93	0.51
1:C:251:ILE:HG22	1:F:100:LEU:HA	1.93	0.51
1:F:87:MET:HE2	7:F:2126:HOH:O	2.09	0.51
1:F:137:PRO:HB2	1:F:204:MET:HE1	1.92	0.51
1:C:336:ARG:N	1:C:336:ARG:HD2	2.28	0.49
1:B:136:VAL:HG12	1:F:302:LEU:HD13	1.94	0.48
1:A:251:ILE:HD12	1:A:296:ALA:HB3	1.95	0.48
1:B:100:LEU:HA	1:F:251:ILE:HG22	1.96	0.48
1:A:39:ILE:HD13	1:A:89:HIS:HB2	1.96	0.47
1:D:20:HIS:CE1	1:D:68:VAL:H	2.33	0.47
1:E:134:GLY:HA2	5:E:1338:ACT:H3	1.95	0.47
1:D:42:LYS:NZ	1:D:60:GLY:O	2.40	0.47
1:B:171:THR:O	1:B:171:THR:HG23	2.15	0.47
1:D:251:ILE:HG22	1:E:100:LEU:HA	1.96	0.47
5:B:1343:ACT:CH3	7:B:2058:HOH:O	2.62	0.46
1:C:73:ASP:OD1	1:C:153:ARG:NH2	2.42	0.46
1:D:247:ARG:HA	1:D:275:TRP:O	2.15	0.46
1:C:66:THR:HA	1:C:147:THR:O	2.16	0.46
1:D:20:HIS:HE1	1:D:68:VAL:H	1.64	0.46
1:A:301:ASN:HA	1:D:243:ASN:O	2.15	0.46
1:B:42:LYS:NZ	1:B:60:GLY:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:PRO:HB2	5:C:1337:ACT:H1	1.98	0.46
1:C:251:ILE:HD12	1:C:296:ALA:HB3	1.97	0.46
1:F:249:HIS:ND1	1:F:273:GLU:O	2.49	0.45
1:A:217:LYS:HG2	1:A:220:ALA:HB2	1.98	0.45
1:D:137:PRO:HB2	1:D:204:MET:CE	2.46	0.45
1:C:301:ASN:HA	1:F:243:ASN:O	2.16	0.45
1:A:294:VAL:HG22	1:A:315:LYS:HG3	1.98	0.44
1:C:332:ALA:HB1	1:C:333:PRO:HD2	1.98	0.44
1:C:336:ARG:NH2	5:E:1338:ACT:O	2.50	0.44
1:E:73:ASP:OD1	1:E:153:ARG:NH2	2.35	0.44
1:B:299:ASN:O	1:B:305:ALA:HB2	2.17	0.44
1:A:136:VAL:HB	1:A:137:PRO:HD3	1.99	0.43
1:A:276:PHE:HB2	1:D:278:ARG:HG2	2.00	0.43
1:F:137:PRO:HB2	1:F:204:MET:CE	2.48	0.43
1:E:202[B]:GLN:NE2	7:E:2178:HOH:O	2.41	0.43
1:B:243:ASN:O	1:F:301:ASN:HA	2.19	0.43
1:D:66:THR:HA	1:D:147:THR:O	2.19	0.43
1:A:249:HIS:ND1	1:A:273:GLU:O	2.52	0.43
1:C:75:VAL:O	1:C:117:ARG:HA	2.19	0.43
5:B:1343:ACT:H1	1:F:270:ARG:HH22	1.84	0.43
1:A:130:CYS:SG	1:A:132:PRO:HD3	2.59	0.42
1:F:154[B]:ASP:CB	4:F:1342:SO4:O2	2.68	0.42
1:E:257:TRP:CZ3	1:E:270:ARG:HB3	2.54	0.42
1:D:298:LEU:C	1:D:298:LEU:HD12	2.40	0.42
1:D:307:GLU:OE2	5:E:1337:ACT:O	2.38	0.42
1:A:137:PRO:HB2	1:A:204:MET:CE	2.50	0.42
1:D:336:ARG:NH1	7:D:2249:HOH:O	2.53	0.42
1:F:56:MET:HB2	1:F:144:MET:HG3	2.01	0.42
1:B:251:ILE:CD1	1:B:296:ALA:HB3	2.46	0.41
1:D:32:VAL:HG22	1:D:74:TYR:HB2	2.02	0.41
1:C:39:ILE:HD13	1:C:89:HIS:HB2	2.02	0.41
1:C:298:LEU:C	1:C:298:LEU:HD12	2.41	0.41
1:F:251:ILE:HD12	1:F:296:ALA:HB3	2.02	0.41
1:F:39:ILE:HD13	1:F:89:HIS:HB2	2.02	0.41
1:C:130:CYS:SG	1:C:132:PRO:HD3	2.61	0.41
1:C:247:ARG:HA	1:C:275:TRP:O	2.21	0.41
1:F:158:ASP:C	1:F:158:ASP:OD1	2.59	0.40
1:C:171:THR:O	1:C:171:THR:HG23	2.21	0.40
1:C:124:GLY:HA2	1:C:264:PHE:CD2	2.56	0.40
1:A:243:ASN:O	1:E:301:ASN:HA	2.21	0.40
1:B:302:LEU:HD13	1:C:136:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:GLU:OE2	5:C:1337:ACT:H2	2.19	0.40
1:D:301:ASN:HA	1:E:243:ASN:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/336 (100%)	328 (98%)	8 (2%)	0	100	100
1	B	334/336 (99%)	326 (98%)	7 (2%)	1 (0%)	41	47
1	C	335/336 (100%)	325 (97%)	10 (3%)	0	100	100
1	D	336/336 (100%)	324 (96%)	12 (4%)	0	100	100
1	E	335/336 (100%)	326 (97%)	9 (3%)	0	100	100
1	F	337/336 (100%)	328 (97%)	8 (2%)	1 (0%)	41	47
All	All	2013/2016 (100%)	1957 (97%)	54 (3%)	2 (0%)	51	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	24	GLN
1	B	24	GLN

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	273/271 (101%)	271 (99%)	2 (1%)	84	90
1	B	270/271 (100%)	266 (98%)	4 (2%)	65	76
1	C	271/271 (100%)	266 (98%)	5 (2%)	59	70
1	D	271/271 (100%)	268 (99%)	3 (1%)	73	83
1	E	271/271 (100%)	268 (99%)	3 (1%)	73	83
1	F	274/271 (101%)	271 (99%)	3 (1%)	73	83
All	All	1630/1626 (100%)	1610 (99%)	20 (1%)	71	82

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
1	A	336	ARG
1	B	9	THR
1	B	168	ARG
1	B	247	ARG
1	B	336	ARG
1	C	4	ASP
1	C	132	PRO
1	C	158	ASP
1	C	168	ARG
1	C	247	ARG
1	D	133	GLU
1	D	158	ASP
1	D	336	ARG
1	E	135	MET
1	E	158	ASP
1	E	336	ARG
1	F	158	ASP
1	F	168	ARG
1	F	275	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	20	HIS
1	D	20	HIS

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 ⓘ

Of 74 ligands modelled in this entry, 12 are monoatomic - leaving 62 for Mogul analysis.

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	SO4	E	1346	-	4,4,4	0.20	0	6,6,6	0.41	0
4	SO4	C	1346	-	4,4,4	0.32	0	6,6,6	0.45	0
6	NO	E	1349	2	0,1,1	0.00	-	-		
4	SO4	A	1347	-	4,4,4	0.18	0	6,6,6	0.52	0
4	SO4	D	1346[B]	-	4,4,4	0.24	0	6,6,6	0.49	0
3	NO2	A	1339	2	1,2,2	4.90	1 (100%)	0,1,1	0.00	-
4	SO4	A	1340	-	4,4,4	0.08	0	6,6,6	0.53	0
4	SO4	F	1346	-	4,4,4	0.22	0	6,6,6	0.35	0
4	SO4	D	1349	-	4,4,4	0.12	0	6,6,6	0.40	0
4	SO4	C	1341	-	4,4,4	0.14	0	6,6,6	0.40	0
5	ACT	B	1343	-	1,3,3	0.73	0	0,3,3	0.00	-
4	SO4	A	1345	-	4,4,4	0.17	0	6,6,6	0.40	0
4	SO4	F	1340	-	4,4,4	0.27	0	6,6,6	0.36	0
5	ACT	A	1341	-	1,3,3	2.89	1 (100%)	0,3,3	0.00	-
5	ACT	D	1339	-	1,3,3	1.66	0	0,3,3	0.00	-
5	ACT	E	1339	-	1,3,3	1.13	0	0,3,3	0.00	-
4	SO4	F	1343	-	4,4,4	0.12	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	F	1344	-	4,4,4	0.28	0	6,6,6	0.51	0
4	SO4	D	1350	-	4,4,4	0.09	0	6,6,6	0.55	0
5	ACT	C	1337	-	1,3,3	0.64	0	0,3,3	0.00	-
4	SO4	A	1344	-	4,4,4	0.15	0	6,6,6	0.56	0
4	SO4	F	1342	-	4,4,4	0.09	0	6,6,6	0.40	0
4	SO4	F	1341	-	4,4,4	0.16	0	6,6,6	0.51	0
4	SO4	B	1344	-	4,4,4	0.30	0	6,6,6	0.21	0
5	ACT	D	1338	-	1,3,3	1.46	0	0,3,3	0.00	-
4	SO4	D	1344	-	4,4,4	0.10	0	6,6,6	0.58	0
4	SO4	B	1348	-	4,4,4	0.17	0	6,6,6	0.26	0
4	SO4	E	1342	-	4,4,4	0.21	0	6,6,6	0.56	0
4	SO4	B	1350	-	4,4,4	0.20	0	6,6,6	0.84	0
3	NO2	B	1341	2	1,2,2	4.61	1 (100%)	0,1,1	0.00	-
4	SO4	B	1347	-	4,4,4	0.18	0	6,6,6	0.16	0
6	NO	C	1347	2	0,1,1	0.00	-	-	-	-
4	SO4	D	1346[A]	-	4,4,4	0.12	0	6,6,6	0.41	0
5	ACT	E	1338	-	1,3,3	0.65	0	0,3,3	0.00	-
5	ACT	E	1337	-	1,3,3	2.72	1 (100%)	0,3,3	0.00	-
4	SO4	E	1347	-	4,4,4	0.12	0	6,6,6	0.54	0
4	SO4	B	1346	-	4,4,4	0.29	0	6,6,6	0.51	0
4	SO4	D	1345	-	4,4,4	0.12	0	6,6,6	0.43	0
4	SO4	C	1345	-	4,4,4	0.21	0	6,6,6	0.63	0
4	SO4	A	1346	-	4,4,4	0.29	0	6,6,6	0.39	0
4	SO4	E	1348	-	4,4,4	0.17	0	6,6,6	0.69	0
4	SO4	D	1337	-	4,4,4	0.26	0	6,6,6	0.59	0
4	SO4	B	1345	-	4,4,4	0.18	0	6,6,6	0.36	0
4	SO4	C	1342	-	4,4,4	0.13	0	6,6,6	0.48	0
3	NO2	A	1342	2	1,2,2	4.58	1 (100%)	0,1,1	0.00	-
3	NO2	F	1339	2	1,2,2	4.93	1 (100%)	0,1,1	0.00	-
4	SO4	E	1343	-	4,4,4	0.19	0	6,6,6	0.41	0
4	SO4	D	1347	-	4,4,4	0.19	0	6,6,6	0.17	0
4	SO4	C	1343	-	4,4,4	0.18	0	6,6,6	0.67	0
4	SO4	B	1340	-	4,4,4	0.16	0	6,6,6	0.37	0
4	SO4	D	1343	-	4,4,4	0.12	0	6,6,6	0.41	0
4	SO4	E	1344	-	4,4,4	0.21	0	6,6,6	0.19	0
4	SO4	B	1349	-	4,4,4	0.23	0	6,6,6	0.37	0
4	SO4	A	1343	-	4,4,4	0.21	0	6,6,6	0.42	0
4	SO4	C	1344	-	4,4,4	0.36	0	6,6,6	0.63	0
4	SO4	A	1348	-	4,4,4	0.14	0	6,6,6	0.17	0
4	SO4	F	1345	-	4,4,4	0.23	0	6,6,6	0.56	0
4	SO4	E	1345	-	4,4,4	0.18	0	6,6,6	0.38	0
5	ACT	B	1342	-	1,3,3	2.41	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	F	1336	-	1,3,3	4.20	1 (100%)	0,3,3	0.00	-
4	SO4	D	1348	-	4,4,4	0.12	0	6,6,6	0.54	0
5	ACT	B	1337	-	1,3,3	1.76	0	0,3,3	0.00	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1339	NO2	O1-N	4.93	1.47	1.22
3	A	1339	NO2	O1-N	4.90	1.47	1.22
3	B	1341	NO2	O1-N	4.61	1.45	1.22
3	A	1342	NO2	O1-N	4.58	1.45	1.22
5	F	1336	ACT	CH3-C	4.20	1.54	1.48
5	A	1341	ACT	CH3-C	2.89	1.52	1.48
5	E	1337	ACT	CH3-C	2.72	1.52	1.48
5	B	1342	ACT	CH3-C	2.41	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1343	ACT	4	0
5	E	1339	ACT	3	0
5	C	1337	ACT	4	0
4	F	1342	SO4	2	0
5	D	1338	ACT	2	0
4	B	1347	SO4	1	0
5	E	1338	ACT	2	0
5	E	1337	ACT	1	0
4	B	1345	SO4	1	0
4	D	1348	SO4	1	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	335/336 (99%)	-0.18	7 (2%)	63	73	28, 37, 54, 74	3 (0%)
1	B	335/336 (99%)	-0.25	6 (1%)	68	76	28, 39, 58, 85	7 (2%)
1	C	335/336 (99%)	-0.22	8 (2%)	59	68	27, 38, 55, 81	4 (1%)
1	D	335/336 (99%)	-0.32	4 (1%)	79	85	28, 39, 57, 77	5 (1%)
1	E	335/336 (99%)	-0.23	10 (2%)	50	60	28, 38, 54, 77	4 (1%)
1	F	334/336 (99%)	-0.28	6 (1%)	68	76	27, 38, 57, 77	4 (1%)
All	All	2009/2016 (99%)	-0.25	41 (2%)	65	74	27, 38, 56, 85	27 (1%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	276	PHE	3.8
1	E	277	ILE	3.7
1	C	276	PHE	3.4
1	A	277	ILE	3.4
1	F	276	PHE	3.3
1	B	276	PHE	3.3
1	A	276	PHE	3.3
1	C	277	ILE	3.2
1	D	276	PHE	3.0
1	C	2	ASP	2.9
1	A	278	ARG	2.8
1	B	2	ASP	2.7
1	D	277	ILE	2.7
1	F	277	ILE	2.7
1	E	4	ASP	2.7
1	C	5	LYS	2.7
1	A	6	LEU	2.7
1	A	5	LYS	2.6
1	F	5	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	277	ILE	2.5
1	B	246	THR	2.4
1	E	2	ASP	2.4
1	B	336	ARG	2.4
1	C	278	ARG	2.4
1	F	183	PRO	2.4
1	E	27	LYS	2.4
1	E	280	GLY	2.3
1	C	4	ASP	2.3
1	E	278	ARG	2.2
1	C	279	GLY	2.2
1	D	335	PRO	2.2
1	E	248	PRO	2.2
1	A	280	GLY	2.2
1	F	25	ALA	2.1
1	B	278	ARG	2.1
1	D	336	ARG	2.1
1	E	275	TRP	2.1
1	F	278	ARG	2.0
1	C	275	TRP	2.0
1	E	281	SER	2.0
1	A	274	THR	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. 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	B-factors(Å ²)	Q<0.9
4	SO4	E	1345	5/5	0.70	0.30	67,69,71,71	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	D	1339	4/4	0.80	0.18	79,80,80,80	0
4	SO4	A	1346	5/5	0.82	0.23	61,62,63,65	5
4	SO4	A	1348	5/5	0.84	0.32	70,70,71,71	5
4	SO4	B	1347	5/5	0.87	0.26	65,65,67,68	5
4	SO4	D	1346[A]	5/5	0.88	0.20	49,50,51,52	5
4	SO4	F	1345	5/5	0.88	0.18	48,50,52,52	5
4	SO4	D	1346[B]	5/5	0.88	0.20	51,52,57,58	5
4	SO4	D	1347	5/5	0.89	0.19	63,64,65,65	5
5	ACT	B	1343	4/4	0.89	0.24	64,64,65,65	0
4	SO4	B	1348	5/5	0.90	0.22	50,54,56,57	5
4	SO4	A	1347	5/5	0.90	0.17	51,56,57,57	5
4	SO4	D	1349	5/5	0.90	0.19	56,59,60,61	5
4	SO4	D	1344	5/5	0.90	0.17	47,49,50,51	5
4	SO4	D	1337	5/5	0.91	0.12	67,68,70,72	5
4	SO4	E	1346	5/5	0.91	0.24	75,75,78,78	5
4	SO4	F	1342	5/5	0.91	0.17	56,57,59,59	5
4	SO4	E	1342	5/5	0.91	0.14	57,58,59,62	4
4	SO4	E	1348	5/5	0.91	0.16	42,44,46,46	5
4	SO4	C	1342	5/5	0.92	0.15	50,50,51,52	5
4	SO4	E	1343	5/5	0.92	0.15	66,68,70,71	5
4	SO4	C	1343	5/5	0.92	0.17	43,46,48,49	5
4	SO4	F	1344	5/5	0.92	0.21	64,66,66,67	5
4	SO4	C	1344	5/5	0.92	0.19	46,48,51,53	5
4	SO4	F	1341	5/5	0.92	0.20	48,50,53,53	5
4	SO4	B	1350	5/5	0.92	0.19	49,50,51,51	5
4	SO4	A	1344	5/5	0.92	0.15	49,50,52,54	5
4	SO4	A	1340	5/5	0.93	0.14	42,42,46,47	5
4	SO4	E	1347	5/5	0.93	0.12	56,58,59,59	5
4	SO4	B	1349	5/5	0.93	0.19	51,51,53,55	5
4	SO4	C	1345	5/5	0.93	0.13	43,48,48,49	5
4	SO4	A	1345	5/5	0.93	0.14	55,56,57,58	5
4	SO4	F	1346	5/5	0.93	0.14	59,60,63,64	5
4	SO4	C	1346	5/5	0.93	0.11	53,56,57,57	5
4	SO4	B	1340	5/5	0.93	0.12	48,49,52,52	5
4	SO4	D	1350	5/5	0.94	0.13	45,45,47,48	5
4	SO4	C	1341	5/5	0.94	0.12	55,56,57,57	5
4	SO4	D	1345	5/5	0.94	0.17	42,44,45,45	5
4	SO4	B	1344	5/5	0.94	0.16	42,44,46,47	5
4	SO4	D	1348	5/5	0.94	0.12	42,44,48,50	5
4	SO4	E	1344	5/5	0.95	0.13	42,44,45,46	5
4	SO4	B	1346	5/5	0.95	0.22	42,45,47,47	5
4	SO4	F	1340	5/5	0.96	0.12	52,52,53,54	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	F	1343	5/5	0.96	0.23	41,45,46,46	5
5	ACT	E	1339	4/4	0.96	0.13	45,46,47,47	4
4	SO4	B	1345	5/5	0.96	0.11	49,49,50,52	5
4	SO4	D	1343	5/5	0.96	0.20	48,50,51,52	5
3	NO2	F	1339	3/3	0.97	0.20	69,69,69,71	0
4	SO4	A	1343	5/5	0.97	0.14	49,49,50,51	5
5	ACT	B	1337	4/4	0.97	0.11	42,42,42,43	0
5	ACT	D	1338	4/4	0.98	0.10	49,49,50,51	0
5	ACT	E	1338	4/4	0.98	0.12	52,53,53,53	0
5	ACT	B	1342	4/4	0.98	0.09	41,42,43,43	0
5	ACT	F	1336	4/4	0.98	0.12	43,44,45,45	0
5	ACT	A	1341	4/4	0.98	0.10	39,40,41,41	0
5	ACT	C	1337	4/4	0.98	0.13	41,42,43,45	0
3	NO2	B	1341	3/3	0.99	0.12	59,59,60,60	0
2	CU	F	1337	1/1	0.99	0.08	35,35,35,35	0
3	NO2	A	1339	3/3	0.99	0.12	57,57,58,60	0
2	CU	E	1340	1/1	0.99	0.09	34,34,34,34	0
6	NO	E	1349	2/2	0.99	0.13	63,63,63,64	0
5	ACT	E	1337	4/4	0.99	0.08	38,40,40,41	0
6	NO	C	1347	2/2	1.00	0.12	45,45,45,46	0
3	NO2	A	1342	3/3	1.00	0.10	69,69,69,70	0
2	CU	D	1340	1/1	1.00	0.08	36,36,36,36	0
2	CU	C	1338	1/1	1.00	0.08	36,36,36,36	0
2	CU	A	1338	1/1	1.00	0.11	35,35,35,35	0
2	CU	B	1339	1/1	1.00	0.10	36,36,36,36	0
2	CU	A	1337	1/1	1.00	0.08	35,35,35,35	0
2	CU	C	1339	1/1	1.00	0.09	35,35,35,35	0
2	CU	F	1338	1/1	1.00	0.11	35,35,35,35	0
2	CU	D	1341	1/1	1.00	0.09	37,37,37,37	0
2	CU	E	1341	1/1	1.00	0.10	36,36,36,36	0
2	CU	B	1338	1/1	1.00	0.09	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.