Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 01:08 am GMT

PDB ID	:	2XX1
Title	:	STRUCTURE OF THE N90S MUTANT OF 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	:	2010-11-07
Resolution	:	3.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

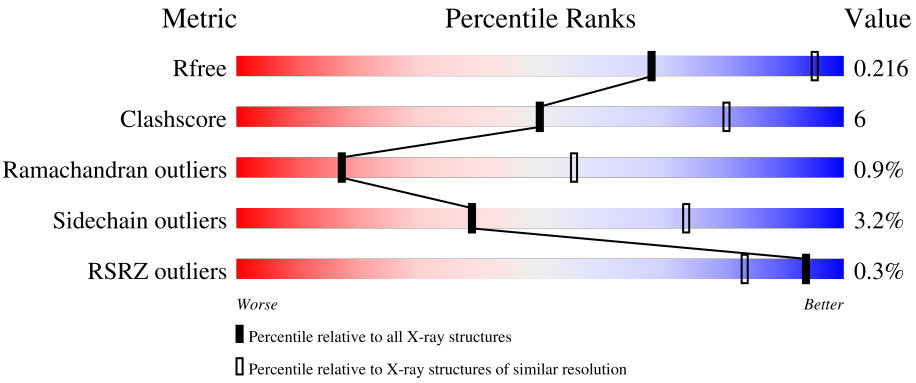
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of 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 <=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	82% 16% ·
1	B	336	% 84% 15% ·
1	C	336	87% 12% ··
1	D	336	84% 15% ·
1	E	336	84% 15%

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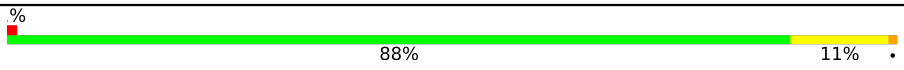
Mol	Chain	Length	Quality of chain
1	F	336	

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
3	NO2	F	1337	-	-	X	-
4	SO4	A	1341	-	-	X	-
4	SO4	A	1343	-	-	-	X
4	SO4	B	1343	-	-	-	X
4	SO4	C	1338	-	-	X	-
4	SO4	E	1345	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15716 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	0	0
			2565	1633	445	476	11			
1	B	335	Total	C	N	O	S	0	0	0
			2565	1633	445	476	11			
1	C	334	Total	C	N	O	S	0	0	0
			2553	1627	441	474	11			
1	D	335	Total	C	N	O	S	0	7	0
			2612	1663	452	485	12			
1	E	335	Total	C	N	O	S	0	0	0
			2565	1633	445	476	11			
1	F	335	Total	C	N	O	S	0	0	0
			2565	1633	445	476	11			

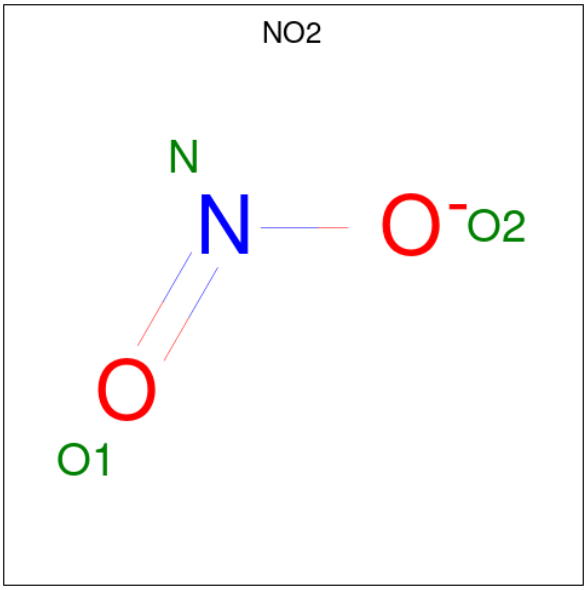
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	expression tag	UNP O68601
A	90	SER	ASN	engineered mutation	UNP O68601
B	1	GLU	-	expression tag	UNP O68601
B	90	SER	ASN	engineered mutation	UNP O68601
C	1	GLU	-	expression tag	UNP O68601
C	90	SER	ASN	engineered mutation	UNP O68601
D	1	GLU	-	expression tag	UNP O68601
D	90	SER	ASN	engineered mutation	UNP O68601
E	1	GLU	-	expression tag	UNP O68601
E	90	SER	ASN	engineered mutation	UNP O68601
F	1	GLU	-	expression tag	UNP O68601
F	90	SER	ASN	engineered mutation	UNP O68601

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

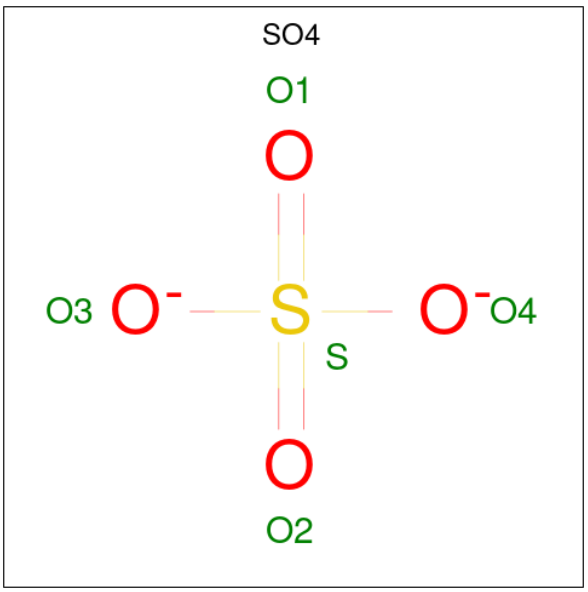
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0
2	E	2	Total Cu 2 2	0	0
2	F	2	Total Cu 2 2	0	0

- Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO_2).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 5 is water.

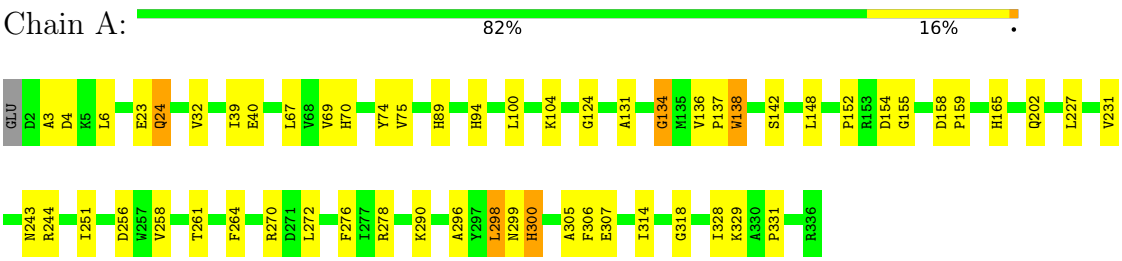
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	22	Total O 22 22	0	0
5	B	31	Total O 31 31	0	0
5	C	29	Total O 29 29	0	0
5	D	18	Total O 18 18	0	0
5	E	31	Total O 31 31	0	0
5	F	25	Total O 25 25	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

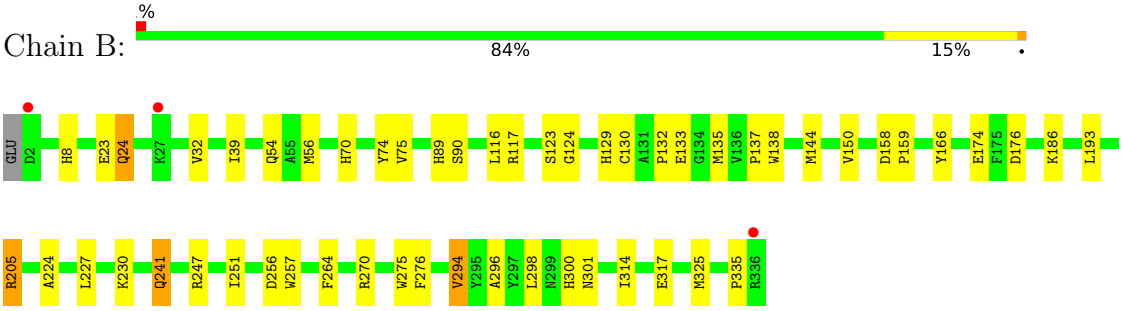
• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain A:



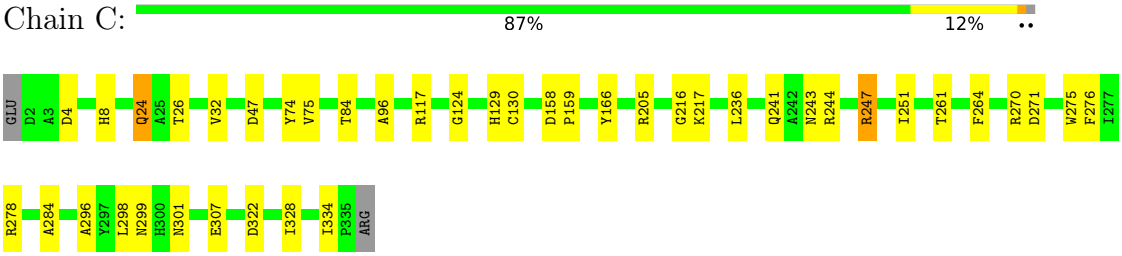
• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain B:



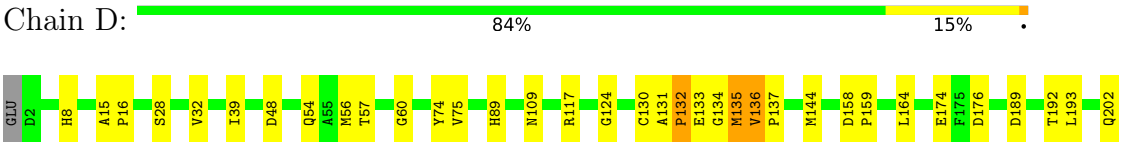
• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain C:



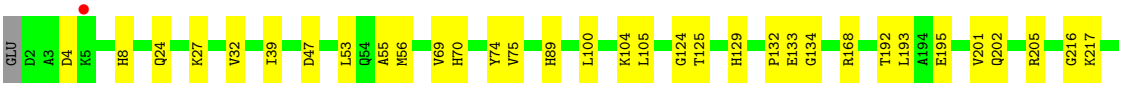
• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain D:



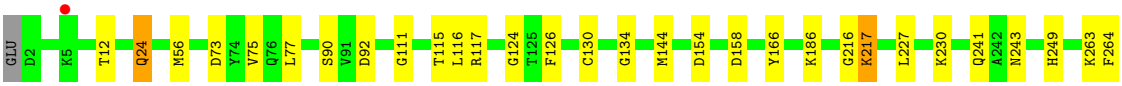
• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain E:



• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	172.67Å 174.65Å 180.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.99 – 3.00 42.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.99-3.00) 99.5 (42.99-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.221 0.181 , 0.216	Depositor DCC
R_{free} test set	5481 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	71.2	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.001 for -h,l,k 0.004 for -l,-k,-h 0.002 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15716	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, NO2, CU

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	0.56	0/2636	0.64	0/3588
1	B	0.53	0/2636	0.66	0/3588
1	C	0.54	0/2624	0.64	0/3574
1	D	0.53	0/2685	0.66	0/3656
1	E	0.52	0/2636	0.65	0/3588
1	F	0.52	0/2636	0.63	0/3588
All	All	0.53	0/15853	0.65	0/21582

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
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) 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

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2565	0	2528	35	0
1	B	2565	0	2527	31	0
1	C	2553	0	2515	26	0
1	D	2612	0	2573	51	0
1	E	2565	0	2528	33	0
1	F	2565	0	2528	22	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	1	0
2	D	2	0	0	1	0
2	E	2	0	0	0	0
2	F	2	0	0	1	0
3	A	3	0	0	0	0
3	B	3	0	0	1	0
3	E	6	0	0	1	0
3	F	6	0	0	2	0
4	A	20	0	0	4	0
4	B	20	0	0	0	0
4	C	20	0	0	5	0
4	D	10	0	0	0	0
4	E	25	0	0	1	0
4	F	10	0	0	0	0
5	A	22	0	0	1	0
5	B	31	0	0	0	0
5	C	29	0	0	1	0
5	D	18	0	0	2	0
5	E	31	0	0	6	0
5	F	25	0	0	1	0
All	All	15716	0	15199	177	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 6.

All (177) 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:D:136[B]:VAL:HB	1:D:137[B]:PRO:HD3	1.34	1.06
1:D:136[A]:VAL:CG2	1:D:136[A]:VAL:O	2.14	0.96
1:D:130:CYS:HG	2:D:1337:CU:CU	0.72	0.96
1:D:136[A]:VAL:O	1:D:136[A]:VAL:HG23	1.64	0.95
1:D:132[A]:PRO:CB	1:D:135[A]:MET:HG2	1.98	0.94
1:F:130:CYS:HG	2:F:1338:CU:CU	0.61	0.92
1:C:130:CYS:HG	2:C:1336:CU:CU	0.61	0.88
1:D:134[B]:GLY:O	1:D:135[B]:MET:HG3	1.74	0.88
1:D:56:MET:O	1:D:144:MET:HG2	1.76	0.86
1:D:132[A]:PRO:HB2	1:D:135[A]:MET:HG2	1.57	0.86
1:D:132[A]:PRO:CB	1:D:135[A]:MET:CG	2.67	0.73
1:B:247:ARG:CZ	4:C:1338:SO4:O4	2.40	0.70
1:D:136[B]:VAL:HB	1:D:137[B]:PRO:CD	2.13	0.69
1:F:124:GLY:HA2	1:F:264:PHE:CD2	2.27	0.69
1:D:32:VAL:HG22	1:D:74:TYR:HB2	1.75	0.69
1:A:307:GLU:OE2	1:D:136[A]:VAL:HB	1.92	0.68
3:B:1339:NO2:O1	1:C:129:HIS:CE1	2.46	0.68
1:E:201:VAL:HG12	4:E:1343:SO4:O3	1.96	0.65
1:E:132:PRO:O	1:E:134:GLY:N	2.30	0.65
1:A:134:GLY:O	5:A:2010:HOH:O	2.14	0.64
1:D:136[B]:VAL:CB	1:D:137[B]:PRO:HD3	2.16	0.64
1:D:54:GLN:HB3	1:D:193:LEU:HD12	1.79	0.64
1:D:132[A]:PRO:HB3	1:D:135[A]:MET:CG	2.30	0.62
1:F:56:MET:O	1:F:144:MET:HG2	2.01	0.61
1:A:276:PHE:HB2	1:D:278:ARG:HG2	1.82	0.61
1:E:251:ILE:HD12	1:E:296:ALA:HB3	1.83	0.60
1:B:251:ILE:HD12	1:B:296:ALA:HB3	1.83	0.60
1:E:56:MET:HE3	1:E:193:LEU:HD11	1.84	0.60
1:A:251:ILE:HD12	1:A:296:ALA:HB3	1.84	0.59
1:B:247:ARG:NH2	4:C:1338:SO4:O4	2.35	0.58
1:A:278:ARG:HG2	1:E:276:PHE:HB2	1.86	0.58
1:E:70:HIS:ND1	5:E:2009:HOH:O	2.32	0.57
1:D:124:GLY:HA2	1:D:264:PHE:CD2	2.40	0.57
1:D:174:GLU:HB3	1:D:241:GLN:HG2	1.87	0.57
1:D:136[B]:VAL:N	1:D:137[B]:PRO:HD2	2.21	0.56
1:A:300:HIS:ND1	1:D:280:GLY:HA3	2.20	0.56
1:A:124:GLY:HA2	1:A:264:PHE:CD2	2.41	0.56
1:B:137:PRO:HG3	1:F:302:LEU:HB2	1.88	0.56
1:D:75:VAL:O	1:D:117:ARG:HA	2.06	0.55
1:D:136[B]:VAL:N	1:D:137[B]:PRO:CD	2.69	0.55
1:C:251:ILE:HD12	1:C:296:ALA:HB3	1.89	0.55
1:A:244:ARG:HG3	4:A:1341:SO4:O1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136[A]:VAL:O	1:D:136[A]:VAL:HG22	2.05	0.55
1:D:136[B]:VAL:CB	1:D:137[B]:PRO:CD	2.81	0.55
1:A:137:PRO:O	1:A:138:TRP:CB	2.55	0.55
1:D:251:ILE:HD12	1:D:296:ALA:HB3	1.89	0.54
1:D:132[A]:PRO:HB3	1:D:135[A]:MET:HG3	1.89	0.54
1:D:158:ASP:HB3	1:D:164:LEU:HD11	1.90	0.54
1:B:137:PRO:HG3	1:F:302:LEU:CB	2.37	0.54
1:A:3:ALA:HA	1:A:6:LEU:HD12	1.90	0.54
1:B:124:GLY:HA2	1:B:264:PHE:CD2	2.42	0.54
1:C:244:ARG:HA	4:C:1338:SO4:O3	2.09	0.53
1:E:336:ARG:NH1	5:E:2030:HOH:O	2.39	0.53
1:E:336:ARG:HD2	1:E:336:ARG:H	1.73	0.53
1:C:247:ARG:HA	1:C:275:TRP:O	2.08	0.53
1:C:301:ASN:HA	1:F:243:ASN:O	2.08	0.53
1:E:124:GLY:HA2	1:E:264:PHE:CD2	2.44	0.53
1:C:124:GLY:HA2	1:C:264:PHE:CD2	2.44	0.53
1:A:328:ILE:HG22	1:A:329:LYS:HG3	1.92	0.52
1:C:32:VAL:HG22	1:C:74:TYR:HB2	1.91	0.52
1:F:24:GLN:NE2	1:F:166:TYR:O	2.43	0.52
1:B:132:PRO:O	1:B:135:MET:HG2	2.10	0.51
1:E:256:ASP:O	1:E:270:ARG:HA	2.11	0.51
1:B:256:ASP:O	1:B:270:ARG:HA	2.09	0.51
1:B:227:LEU:HB2	1:B:314:ILE:HG12	1.91	0.50
1:D:251:ILE:HG22	1:E:100:LEU:HA	1.93	0.50
1:C:244:ARG:HG3	4:C:1338:SO4:O3	2.11	0.50
1:A:67:LEU:O	1:A:148:LEU:HD12	2.12	0.50
4:A:1341:SO4:O3	1:E:247:ARG:NH2	2.45	0.50
1:B:129:HIS:CE1	3:F:1337:NO2:O1	2.65	0.50
1:C:236:LEU:HD11	1:C:284:ALA:HB1	1.93	0.50
1:A:244:ARG:HA	4:A:1341:SO4:O1	2.12	0.49
1:D:48:ASP:HB2	5:D:2004:HOH:O	2.12	0.49
1:E:32:VAL:HG22	1:E:74:TYR:HB2	1.93	0.49
1:E:39:ILE:HG21	1:E:89:HIS:CD2	2.47	0.49
1:D:301:ASN:HA	1:E:243:ASN:O	2.12	0.49
1:E:227:LEU:HB2	1:E:314:ILE:HG12	1.94	0.49
1:A:24:GLN:HE22	1:A:165:HIS:HA	1.76	0.49
1:C:24:GLN:HE22	1:C:166:TYR:H	1.60	0.49
1:A:137:PRO:O	1:A:138:TRP:HB2	2.12	0.49
4:A:1341:SO4:O3	1:E:247:ARG:CZ	2.61	0.48
1:E:27:LYS:HB2	5:E:2003:HOH:O	2.13	0.48
1:C:158:ASP:HB2	1:C:159:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG22	1:A:74:TYR:HB2	1.96	0.48
1:E:202:GLN:HG3	5:E:2031:HOH:O	2.14	0.48
1:B:129:HIS:HE1	3:F:1337:NO2:O1	1.97	0.47
1:C:276:PHE:HB2	1:F:278:ARG:HG2	1.95	0.47
1:B:174:GLU:HB3	1:B:241:GLN:HG2	1.95	0.47
1:A:243:ASN:O	1:E:301:ASN:HA	2.14	0.47
1:D:130:CYS:SG	1:D:132[B]:PRO:HD3	2.55	0.47
1:C:270:ARG:O	1:C:271:ASP:HB2	2.14	0.47
1:E:277:ILE:HD12	1:E:283:GLY:HA3	1.97	0.47
1:A:158:ASP:HB2	1:A:159:PRO:CD	2.45	0.47
1:B:276:PHE:HB2	1:C:278:ARG:HG2	1.98	0.47
1:E:47:ASP:HB2	5:E:2006:HOH:O	2.15	0.47
1:D:39:ILE:HD13	1:D:89:HIS:HB2	1.97	0.46
1:D:132[A]:PRO:CA	1:D:135[A]:MET:HG2	2.45	0.46
1:B:75:VAL:O	1:B:117:ARG:HA	2.14	0.46
1:F:75:VAL:O	1:F:117:ARG:HA	2.15	0.46
1:D:131[A]:ALA:HA	1:D:132[A]:PRO:HD3	1.73	0.46
1:A:100:LEU:HA	1:E:251:ILE:HG22	1.97	0.46
1:D:158:ASP:HB2	1:D:159:PRO:HD3	1.96	0.46
1:D:131[B]:ALA:O	1:D:132[B]:PRO:O	2.33	0.46
1:F:249:HIS:ND1	1:F:273:GLU:O	2.49	0.46
1:B:123:SER:HA	1:B:150:VAL:HG12	1.97	0.45
1:E:216:GLY:O	1:E:217:LYS:HB3	2.17	0.45
1:F:227:LEU:HB2	1:F:314:ILE:HG12	1.99	0.45
1:D:136[A]:VAL:HA	1:D:137[A]:PRO:HD2	1.66	0.45
1:A:39:ILE:HD13	1:A:89:HIS:HB2	1.99	0.45
1:A:258:VAL:HB	1:A:272:LEU:HD12	1.98	0.45
1:D:256:ASP:O	1:D:270:ARG:HA	2.16	0.45
1:C:241:GLN:NE2	1:C:244:ARG:HB3	2.32	0.45
1:E:251:ILE:CD1	1:E:296:ALA:HB3	2.45	0.44
1:A:138:TRP:O	1:A:142:SER:OG	2.28	0.44
1:A:227:LEU:HB2	1:A:314:ILE:HG12	1.99	0.44
1:D:15:ALA:HA	1:D:16:PRO:HD3	1.88	0.44
1:D:109:ASN:HD22	1:D:109:ASN:N	2.16	0.44
1:E:329:LYS:NZ	5:E:2029:HOH:O	2.50	0.44
1:A:94:HIS:CD2	1:E:249:HIS:CE1	3.05	0.44
1:B:301:ASN:HA	1:C:243:ASN:O	2.18	0.44
1:D:158:ASP:HB2	1:D:159:PRO:CD	2.47	0.44
1:A:251:ILE:HD11	1:A:298:LEU:HD21	1.99	0.44
1:E:69:VAL:HG11	1:E:75:VAL:HG22	2.00	0.44
1:C:251:ILE:CD1	1:C:296:ALA:HB3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:VAL:HG12	1:B:294:VAL:O	2.17	0.43
1:F:77:LEU:O	1:F:115:THR:HA	2.19	0.43
1:B:176:ASP:OD1	1:B:176:ASP:N	2.47	0.43
1:E:231:VAL:HG23	1:E:317:GLU:O	2.18	0.43
1:A:299:ASN:O	1:A:305:ALA:HB2	2.19	0.43
1:C:216:GLY:O	1:C:217:LYS:HB3	2.19	0.43
1:F:126:PHE:CE2	1:F:263:LYS:HE3	2.54	0.43
1:F:216:GLY:O	1:F:217:LYS:HB3	2.20	0.42
1:C:75:VAL:O	1:C:117:ARG:HA	2.19	0.42
1:C:244:ARG:CG	4:C:1338:SO4:O3	2.68	0.42
1:B:56:MET:O	1:B:144:MET:HG2	2.19	0.42
1:C:328:ILE:HG12	1:F:117:ARG:HB2	2.01	0.42
1:B:90:SER:O	1:B:130:CYS:HA	2.20	0.42
1:A:306:PHE:CE1	1:D:134[A]:GLY:HA2	2.54	0.42
1:E:53:LEU:HD23	1:E:55:ALA:HB2	2.01	0.42
1:F:300:HIS:O	1:F:300:HIS:ND1	2.49	0.42
1:B:23:GLU:O	1:B:70:HIS:NE2	2.53	0.42
1:D:259:TRP:CE2	1:D:268:PRO:HB3	2.55	0.42
1:B:32:VAL:HG22	1:B:74:TYR:HB2	2.02	0.41
1:C:334:ILE:HG13	1:F:111:GLY:O	2.21	0.41
1:F:90:SER:O	1:F:130:CYS:HA	2.20	0.41
1:A:152:PRO:HG2	1:A:155:GLY:O	2.20	0.41
1:D:57:THR:OG1	1:D:60:GLY:HA2	2.20	0.41
5:D:2013:HOH:O	1:E:104:LYS:HE2	2.19	0.41
1:B:230:LYS:HB3	1:B:317:GLU:HB2	2.02	0.41
1:B:257:TRP:CZ3	1:B:270:ARG:HB3	2.56	0.41
1:D:132[A]:PRO:HB2	1:D:135[A]:MET:H	1.86	0.41
1:D:263:LYS:HA	1:D:263:LYS:HD3	1.96	0.41
1:A:158:ASP:CB	1:A:159:PRO:CD	2.99	0.41
1:D:132[A]:PRO:HB2	1:D:135[A]:MET:CG	2.39	0.41
1:F:134:GLY:O	5:F:2012:HOH:O	2.22	0.41
1:A:270:ARG:HD3	1:D:265:ALA:HB1	2.01	0.41
1:B:247:ARG:HA	1:B:275:TRP:O	2.21	0.41
1:E:129:HIS:CE1	3:E:1340:NO2:O1	2.73	0.41
1:A:69:VAL:HG11	1:A:75:VAL:HG22	2.02	0.41
1:B:325:MET:CE	1:C:96:ALA:HB1	2.50	0.41
1:B:54:GLN:HB3	1:B:193:LEU:HD12	2.03	0.41
1:B:158:ASP:HB2	1:B:159:PRO:CD	2.51	0.41
1:B:205:ARG:HG2	1:F:307:GLU:OE2	2.21	0.41
1:C:299:ASN:OD1	1:C:299:ASN:C	2.59	0.41
1:D:231:VAL:HG23	1:D:318:GLY:HA3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:TRP:CZ3	1:D:270:ARG:HB3	2.56	0.40
1:F:92:ASP:C	1:F:92:ASP:OD1	2.59	0.40
1:A:256:ASP:O	1:A:270:ARG:HA	2.22	0.40
1:B:39:ILE:HD13	1:B:89:HIS:HB2	2.03	0.40
1:C:47:ASP:HB2	5:C:2002:HOH:O	2.20	0.40
1:A:23:GLU:O	1:A:70:HIS:NE2	2.53	0.40
1:B:24:GLN:HE22	1:B:166:TYR:H	1.68	0.40
1:E:192:THR:OG1	1:E:195:GLU:HG3	2.21	0.40
1:A:131:ALA:HA	1:A:136:VAL:HG13	2.04	0.40
1:A:231:VAL:HG23	1:A:318:GLY:HA3	2.04	0.40
1:D:132[B]:PRO:HB2	1:D:133[B]:GLU:H	1.63	0.40
1:F:263:LYS:HD3	1:F:263:LYS:HA	1.87	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	333/336 (99%)	317 (95%)	12 (4%)	4 (1%)	13	48
1	B	333/336 (99%)	315 (95%)	14 (4%)	4 (1%)	13	48
1	C	332/336 (99%)	318 (96%)	13 (4%)	1 (0%)	41	76
1	D	340/336 (101%)	314 (92%)	20 (6%)	6 (2%)	8	37
1	E	333/336 (99%)	317 (95%)	14 (4%)	2 (1%)	25	64
1	F	333/336 (99%)	313 (94%)	17 (5%)	3 (1%)	17	55
All	All	2004/2016 (99%)	1894 (94%)	90 (4%)	20 (1%)	17	53

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	TRP

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Mol	Chain	Res	Type
1	B	138	TRP
1	B	335	PRO
1	D	132[A]	PRO
1	D	132[B]	PRO
1	A	24	GLN
1	A	134	GLY
1	B	224	ALA
1	F	335	PRO
1	B	24	GLN
1	D	28	SER
1	E	24	GLN
1	F	24	GLN
1	C	24	GLN
1	D	135[A]	MET
1	D	135[B]	MET
1	E	133	GLU
1	F	73	ASP
1	D	335	PRO
1	A	331	PRO

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	270/271 (100%)	262 (97%)	8 (3%)	41	75
1	B	270/271 (100%)	262 (97%)	8 (3%)	41	75
1	C	269/271 (99%)	259 (96%)	10 (4%)	34	70
1	D	275/271 (102%)	267 (97%)	8 (3%)	42	76
1	E	270/271 (100%)	262 (97%)	8 (3%)	41	75
1	F	270/271 (100%)	260 (96%)	10 (4%)	34	70
All	All	1624/1626 (100%)	1572 (97%)	52 (3%)	39	74

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	40	GLU
1	A	104	LYS
1	A	154	ASP
1	A	202	GLN
1	A	261	THR
1	A	290	LYS
1	A	298	LEU
1	B	8	HIS
1	B	116	LEU
1	B	133	GLU
1	B	186	LYS
1	B	205	ARG
1	B	241	GLN
1	B	294	VAL
1	B	298	LEU
1	C	4	ASP
1	C	8	HIS
1	C	26	THR
1	C	84	THR
1	C	205	ARG
1	C	247	ARG
1	C	261	THR
1	C	298	LEU
1	C	307	GLU
1	C	322	ASP
1	D	8	HIS
1	D	136[A]	VAL
1	D	136[B]	VAL
1	D	176	ASP
1	D	189	ASP
1	D	192	THR
1	D	202	GLN
1	D	298	LEU
1	E	4	ASP
1	E	8	HIS
1	E	105	LEU
1	E	125	THR
1	E	168	ARG
1	E	205	ARG
1	E	298	LEU
1	E	336	ARG
1	F	12	THR

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Mol	Chain	Res	Type
1	F	116	LEU
1	F	154	ASP
1	F	158	ASP
1	F	186	LYS
1	F	217	LYS
1	F	230	LYS
1	F	241	GLN
1	F	275	TRP
1	F	298	LEU

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

Mol	Chain	Res	Type
1	A	165	HIS
1	D	109	ASN
1	F	327	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 12 are monoatomic - leaving 27 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	$\#\|Z\|>2$
3	NO2	F	1337	2	1,2,2	4.41	1 (100%)	0,1,1	-	-
4	SO4	A	1342	-	4,4,4	0.15	0	6,6,6	0.33	0
4	SO4	D	1340	-	4,4,4	0.14	0	6,6,6	0.18	0
4	SO4	A	1343	-	4,4,4	0.14	0	6,6,6	0.21	0
4	SO4	F	1342	-	4,4,4	0.16	0	6,6,6	0.19	0
3	NO2	F	1340	2	1,2,2	4.39	1 (100%)	0,1,1	-	-
4	SO4	C	1338	-	4,4,4	0.39	0	6,6,6	0.78	0
4	SO4	E	1345	-	4,4,4	0.11	0	6,6,6	0.19	0
4	SO4	B	1343	-	4,4,4	0.18	0	6,6,6	0.18	0
4	SO4	E	1341	-	4,4,4	0.12	0	6,6,6	0.22	0
4	SO4	B	1342	-	4,4,4	0.11	0	6,6,6	0.18	0
3	NO2	E	1340	2	1,2,2	4.43	1 (100%)	0,1,1	-	-
4	SO4	E	1343	-	4,4,4	0.21	0	6,6,6	0.54	0
3	NO2	E	1337	2	1,2,2	4.58	1 (100%)	0,1,1	-	-
3	NO2	A	1339	2	1,2,2	4.50	1 (100%)	0,1,1	-	-
4	SO4	E	1342	-	4,4,4	0.17	0	6,6,6	0.27	0
4	SO4	C	1339	-	4,4,4	0.16	0	6,6,6	0.22	0
4	SO4	F	1341	-	4,4,4	0.15	0	6,6,6	0.24	0
3	NO2	B	1339	2	1,2,2	4.40	1 (100%)	0,1,1	-	-
4	SO4	B	1341	-	4,4,4	0.14	0	6,6,6	0.22	0
4	SO4	D	1339	-	4,4,4	0.15	0	6,6,6	0.22	0
4	SO4	A	1341	-	4,4,4	0.23	0	6,6,6	0.50	0
4	SO4	E	1344	-	4,4,4	0.17	0	6,6,6	0.16	0
4	SO4	C	1340	-	4,4,4	0.14	0	6,6,6	0.19	0
4	SO4	B	1340	-	4,4,4	0.19	0	6,6,6	0.34	0
4	SO4	C	1341	-	4,4,4	0.11	0	6,6,6	0.16	0
4	SO4	A	1340	-	4,4,4	0.13	0	6,6,6	0.10	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1337	NO2	O1-N	4.58	1.45	1.22
3	A	1339	NO2	O1-N	4.50	1.45	1.22
3	E	1340	NO2	O1-N	4.43	1.44	1.22
3	F	1337	NO2	O1-N	4.41	1.44	1.22
3	B	1339	NO2	O1-N	4.40	1.44	1.22
3	F	1340	NO2	O1-N	4.39	1.44	1.22

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1337	NO2	2	0
4	C	1338	SO4	5	0
3	E	1340	NO2	1	0
4	E	1343	SO4	1	0
3	B	1339	NO2	1	0
4	A	1341	SO4	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.30	0 100 100	49, 66, 90, 112	1 (0%)
1	B	335/336 (99%)	-0.32	3 (0%) 84 63	47, 66, 89, 112	0
1	C	334/336 (99%)	-0.32	0 100 100	50, 66, 87, 113	1 (0%)
1	D	335/336 (99%)	-0.35	1 (0%) 94 84	49, 67, 88, 113	1 (0%)
1	E	335/336 (99%)	-0.32	1 (0%) 94 84	48, 65, 86, 110	1 (0%)
1	F	335/336 (99%)	-0.37	2 (0%) 89 72	49, 66, 89, 112	0
All	All	2009/2016 (99%)	-0.33	7 (0%) 94 84	47, 66, 89, 113	4 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	336	ARG	2.9
1	D	336	ARG	2.8
1	B	2	ASP	2.3
1	B	336	ARG	2.3
1	E	5	LYS	2.2
1	B	27	LYS	2.1
1	F	5	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides 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, 95^{th} 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	0.61	0.41	92,93,93,93	5
4	SO4	B	1343	5/5	0.67	0.40	78,78,79,79	5
4	SO4	A	1343	5/5	0.73	0.42	74,74,75,75	5
4	SO4	E	1344	5/5	0.74	0.34	78,78,79,79	5
4	SO4	B	1342	5/5	0.81	0.33	76,77,77,78	5
4	SO4	D	1339	5/5	0.82	0.41	72,72,72,73	5
4	SO4	C	1338	5/5	0.83	0.43	43,45,45,46	5
4	SO4	E	1343	5/5	0.83	0.52	60,61,62,63	5
4	SO4	E	1342	5/5	0.84	0.29	67,67,67,68	5
4	SO4	C	1340	5/5	0.85	0.35	63,64,64,64	5
4	SO4	F	1342	5/5	0.87	0.36	67,67,68,68	5
4	SO4	F	1341	5/5	0.88	0.29	72,73,73,74	5
4	SO4	B	1340	5/5	0.88	0.41	58,58,60,60	5
4	SO4	C	1341	5/5	0.89	0.25	74,74,75,75	5
4	SO4	B	1341	5/5	0.89	0.26	62,63,63,63	5
4	SO4	A	1342	5/5	0.90	0.26	70,71,72,73	5
4	SO4	E	1341	5/5	0.90	0.23	61,61,61,62	5
4	SO4	D	1340	5/5	0.91	0.25	71,71,72,72	5
4	SO4	A	1341	5/5	0.91	0.46	46,46,47,48	5
4	SO4	A	1340	5/5	0.92	0.26	71,71,71,72	5
4	SO4	C	1339	5/5	0.94	0.24	60,61,62,62	5
2	CU	D	1337	1/1	0.99	0.09	85,85,85,85	1
2	CU	E	1338	1/1	0.99	0.13	49,49,49,49	1
2	CU	F	1338	1/1	0.99	0.07	116,116,116,116	0
2	CU	A	1337	1/1	0.99	0.14	77,77,77,77	1
2	CU	B	1337	1/1	0.99	0.15	66,66,66,66	1
2	CU	C	1336	1/1	0.99	0.16	65,65,65,65	1
3	NO2	E	1340	3/3	1.00	0.17	56,56,56,57	0
3	NO2	F	1337	3/3	1.00	0.18	58,58,59,59	0
3	NO2	F	1340	3/3	1.00	0.17	72,72,73,73	0
2	CU	B	1338	1/1	1.00	0.15	55,55,55,55	0
2	CU	D	1338	1/1	1.00	0.16	58,58,58,58	0
2	CU	A	1338	1/1	1.00	0.18	53,53,53,53	0
2	CU	E	1339	1/1	1.00	0.16	57,57,57,57	0
2	CU	C	1337	1/1	1.00	0.18	60,60,60,60	0
2	CU	F	1339	1/1	1.00	0.15	54,54,54,54	0
3	NO2	A	1339	3/3	1.00	0.18	63,63,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NO2	B	1339	3/3	1.00	0.20	49,49,49,50	0
3	NO2	E	1337	3/3	1.00	0.15	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.