



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:53 AM UTC

PDB ID : 2XX1 / pdb_00002xx1
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

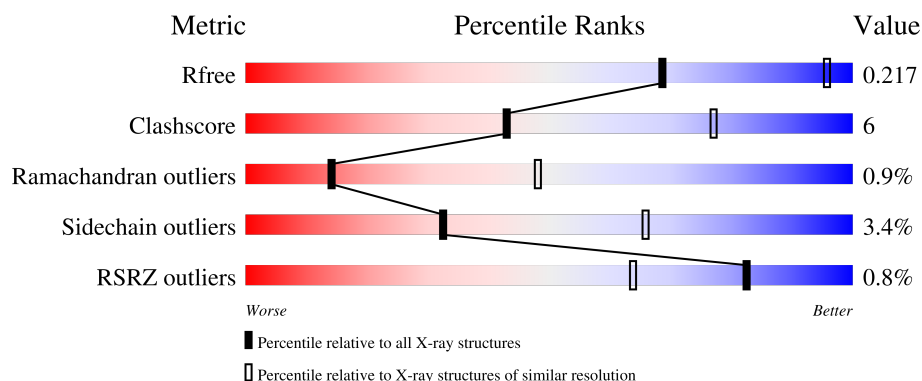
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	2% 82% 17%
1	B	336	82% 16%
1	C	336	86% 12%
1	D	336	2% 83% 15%
1	E	336	2% 83% 16%

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Mol	Chain	Length	Quality of chain
1	F	336	% 86% 13%

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	C	1338	-	-	X	-

2 Entry composition

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			

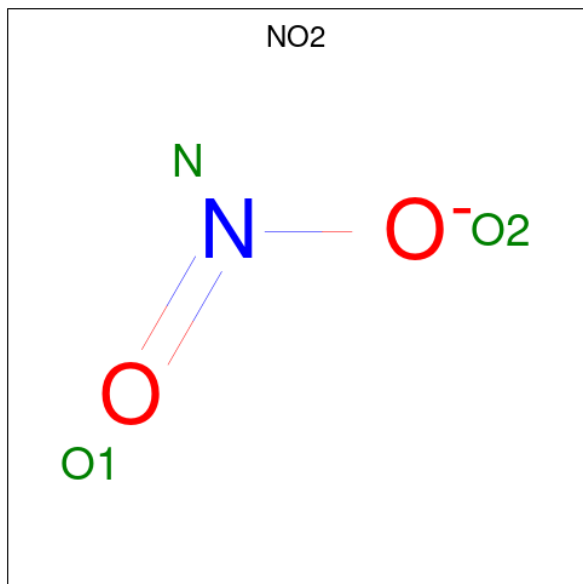
There are 12 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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 (CCD ID: NO2) (formula: NO₂).



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 (CCD ID: 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	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	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		

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

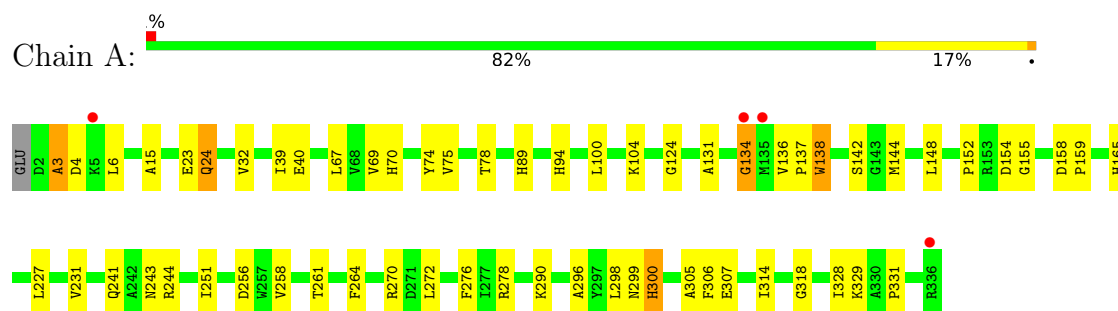
- Molecule 5 is water.

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

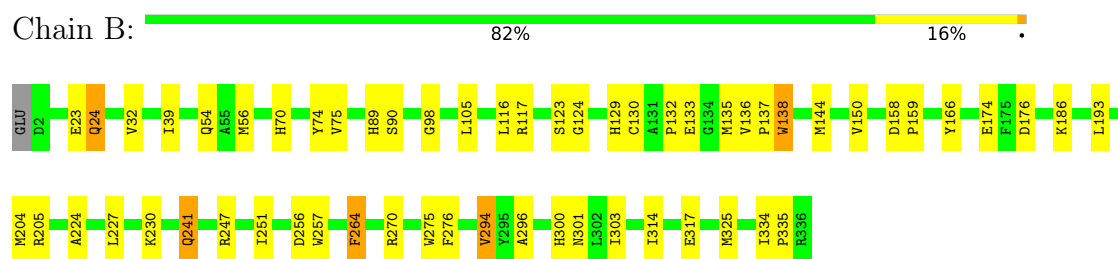
3 Residue-property plots [i](#)

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.

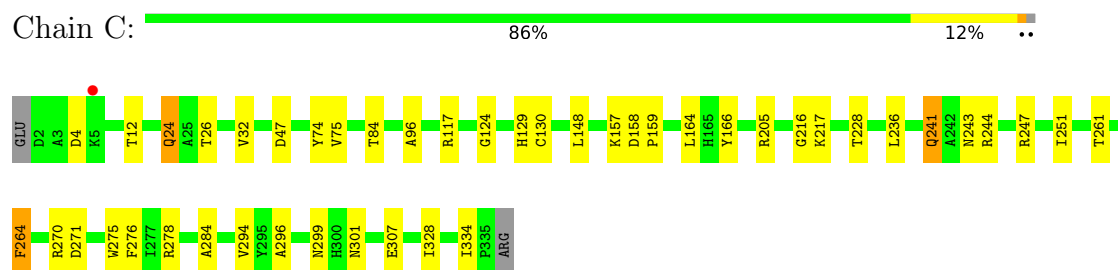
• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE



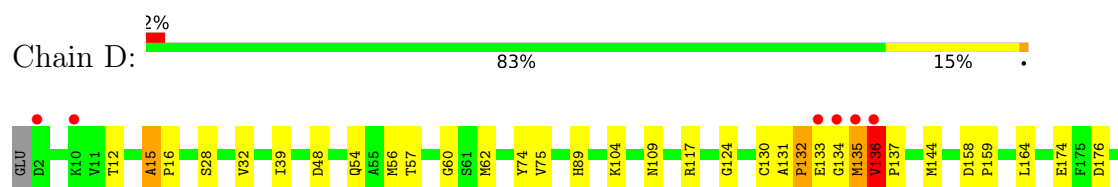
• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

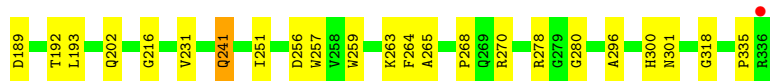


• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

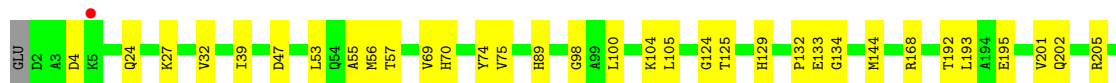
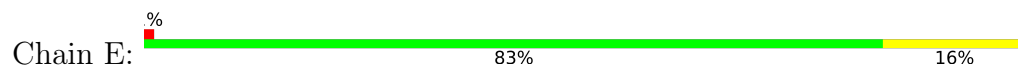


• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

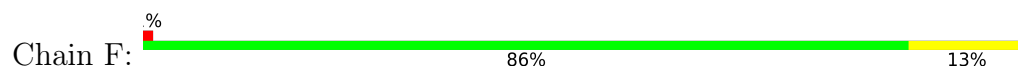




- Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE



- Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE



4 Data and refinement statistics

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) 99.6 (42.99-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.221 0.181 , 0.217	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)	0.32 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, SO4, NO2

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	0.69	0/2636	0.92	3/3588 (0.1%)
1	B	0.66	0/2636	0.95	7/3588 (0.2%)
1	C	0.65	0/2624	0.90	1/3574 (0.0%)
1	D	0.65	0/2685	0.94	6/3656 (0.2%)
1	E	0.64	0/2636	0.90	1/3588 (0.0%)
1	F	0.66	0/2636	0.91	5/3588 (0.1%)
All	All	0.66	0/15853	0.92	23/21582 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	136[A]	VAL	CA-C-N	7.00	128.59	119.84
1	D	136[A]	VAL	C-N-CA	7.00	128.59	119.84
1	D	136[B]	VAL	CA-C-N	7.00	128.59	119.84
1	D	136[B]	VAL	C-N-CA	7.00	128.59	119.84
1	F	334	ILE	CA-C-N	6.62	128.11	119.84
1	F	334	ILE	C-N-CA	6.62	128.11	119.84
1	B	334	ILE	CA-C-N	6.44	127.89	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	ILE	C-N-CA	6.44	127.89	119.84
1	A	3	ALA	N-CA-C	6.08	118.82	111.40
1	B	303	ILE	N-CA-C	-6.08	104.82	110.53
1	B	136	VAL	CA-C-N	6.05	127.41	119.84
1	B	136	VAL	C-N-CA	6.05	127.41	119.84
1	B	264	PHE	N-CA-C	5.92	118.69	111.82
1	B	98	GLY	N-CA-C	5.77	117.43	111.95
1	A	15	ALA	CA-C-N	5.74	126.29	120.38
1	A	15	ALA	C-N-CA	5.74	126.29	120.38
1	E	98	GLY	N-CA-C	5.49	118.91	111.72
1	F	64	GLY	CA-C-N	-5.44	114.64	120.03
1	F	64	GLY	C-N-CA	-5.44	114.64	120.03
1	D	15	ALA	CA-C-N	5.42	125.97	120.38
1	D	15	ALA	C-N-CA	5.42	125.97	120.38
1	C	264	PHE	N-CA-C	5.37	118.05	111.82
1	F	217	LYS	N-CA-C	5.13	116.33	108.42

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	36	0
1	B	2565	0	2527	34	0
1	C	2553	0	2515	27	0
1	D	2612	0	2573	54	0
1	E	2565	0	2528	34	0
1	F	2565	0	2528	24	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	187	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 (187) 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: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	0.91
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:MET:HE2	1:E:193:LEU:HD21	1.83	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:A:251:ILE:HD12	1:A:296:ALA:HB3	1.84	0.59
1:D:62:MET:HE2	1:D:216:GLY:HA2	1.85	0.58
1:B:247:ARG:NH2	4:C:1338:SO4:O4	2.35	0.58
1:D:56:MET:HE2	1:D:193:LEU:HD21	1.85	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:130:CYS:HG	2:D:1337:CU:CU	1.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:57:THR:C	1:F:144:MET:HE3	2.34	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:B:325:MET:HE2	1:C:96:ALA:HB1	1.92	0.52
1:F:24:GLN:NE2	1:F:166:TYR:O	2.43	0.52
1:B:56:MET:HE2	1:B:193:LEU:HD21	1.91	0.51
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:D:134[B]:GLY:C	1:D:135[B]:MET:HG3	2.38	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
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:A:39:ILE:HG12	1:A:144:MET:HE1	1.97	0.47
1:B:174:GLU:HB3	1:B:241:GLN:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:299:ASN:OD1	1:C:299:ASN:C	2.59	0.45
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:F:92:ASP:OD1	1:F:92:ASP:C	2.59	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:138:TRP:H	1:B:204:MET:HE1	1.84	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:D:231:VAL:HG23	1:D:318:GLY:HA3	2.02	0.40
1:D:257:TRP:CZ3	1:D:270:ARG:HB3	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:57:THR:C	1:E:144:MET:HE3	2.46	0.40
1:F:321:ASN:OD1	1:F:321:ASN:C	2.63	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%)	10	40
1	B	333/336 (99%)	315 (95%)	14 (4%)	4 (1%)	10	40
1	C	332/336 (99%)	318 (96%)	13 (4%)	1 (0%)	36	70
1	D	340/336 (101%)	314 (92%)	20 (6%)	6 (2%)	6	31
1	E	333/336 (99%)	317 (95%)	14 (4%)	2 (1%)	21	56
1	F	333/336 (99%)	313 (94%)	17 (5%)	3 (1%)	14	48
All	All	2004/2016 (99%)	1894 (94%)	90 (4%)	20 (1%)	14	45

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	TRP
1	B	138	TRP

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Mol	Chain	Res	Type
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 ⓘ

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%)	36	69
1	B	270/271 (100%)	264 (98%)	6 (2%)	45	74
1	C	269/271 (99%)	256 (95%)	13 (5%)	23	57
1	D	275/271 (102%)	266 (97%)	9 (3%)	33	67
1	E	270/271 (100%)	262 (97%)	8 (3%)	36	69
1	F	270/271 (100%)	258 (96%)	12 (4%)	25	60
All	All	1624/1626 (100%)	1568 (97%)	56 (3%)	32	66

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	40	GLU
1	A	78	THR
1	A	104	LYS
1	A	154	ASP
1	A	241	GLN
1	A	261	THR
1	A	290	LYS
1	B	105	LEU
1	B	116	LEU
1	B	133	GLU
1	B	186	LYS
1	B	241	GLN
1	B	294	VAL
1	C	4	ASP
1	C	12	THR
1	C	26	THR
1	C	84	THR
1	C	148	LEU
1	C	157	LYS
1	C	164	LEU
1	C	205	ARG
1	C	228	THR
1	C	241	GLN
1	C	261	THR
1	C	294	VAL
1	C	307	GLU
1	D	12	THR
1	D	104	LYS
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	241	GLN
1	E	4	ASP
1	E	105	LEU
1	E	125	THR
1	E	168	ARG
1	E	205	ARG
1	E	275	TRP
1	E	290	LYS

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Mol	Chain	Res	Type
1	E	336	ARG
1	F	12	THR
1	F	116	LEU
1	F	154	ASP
1	F	157	LYS
1	F	186	LYS
1	F	217	LYS
1	F	230	LYS
1	F	241	GLN
1	F	275	TRP
1	F	294	VAL
1	F	298	LEU
1	F	336	ARG

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

Mol	Chain	Res	Type
1	A	113	GLN
1	A	165	HIS
1	B	76	GLN
1	C	18	GLN
1	C	85	ASN
1	C	139	HIS
1	D	109	ASN
1	D	269	GLN
1	E	76	GLN
1	E	107	ASN
1	E	139	HIS
1	F	113	GLN
1	F	139	HIS
1	F	269	GLN
1	F	327	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 [i](#)

There are no oligosaccharides 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
4	SO4	F	1342	-	4,4,4	0.27	0	6,6,6	0.18	0
4	SO4	A	1341	-	4,4,4	0.29	0	6,6,6	0.52	0
4	SO4	E	1343	-	4,4,4	0.31	0	6,6,6	0.45	0
4	SO4	F	1341	-	4,4,4	0.26	0	6,6,6	0.24	0
3	NO2	B	1339	2	1,2,2	4.45	1 (100%)	0,1,1	-	-
3	NO2	E	1340	2	1,2,2	4.48	1 (100%)	0,1,1	-	-
4	SO4	B	1340	-	4,4,4	0.30	0	6,6,6	0.35	0
4	SO4	E	1342	-	4,4,4	0.29	0	6,6,6	0.30	0
4	SO4	C	1338	-	4,4,4	0.48	0	6,6,6	0.62	0
4	SO4	C	1339	-	4,4,4	0.28	0	6,6,6	0.24	0
3	NO2	A	1339	2	1,2,2	4.55	1 (100%)	0,1,1	-	-
4	SO4	D	1340	-	4,4,4	0.26	0	6,6,6	0.19	0
4	SO4	A	1343	-	4,4,4	0.25	0	6,6,6	0.15	0
4	SO4	A	1340	-	4,4,4	0.24	0	6,6,6	0.10	0
4	SO4	B	1341	-	4,4,4	0.25	0	6,6,6	0.17	0
4	SO4	C	1340	-	4,4,4	0.25	0	6,6,6	0.17	0
4	SO4	E	1341	-	4,4,4	0.22	0	6,6,6	0.20	0
4	SO4	A	1342	-	4,4,4	0.26	0	6,6,6	0.34	0
3	NO2	E	1337	2	1,2,2	4.63	1 (100%)	0,1,1	-	-
3	NO2	F	1340	2	1,2,2	4.43	1 (100%)	0,1,1	-	-
4	SO4	D	1339	-	4,4,4	0.27	0	6,6,6	0.26	0
4	SO4	E	1345	-	4,4,4	0.22	0	6,6,6	0.17	0
4	SO4	C	1341	-	4,4,4	0.20	0	6,6,6	0.13	0
3	NO2	F	1337	2	1,2,2	4.46	1 (100%)	0,1,1	-	-
4	SO4	B	1342	-	4,4,4	0.22	0	6,6,6	0.18	0
4	SO4	E	1344	-	4,4,4	0.28	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	1343	-	4,4,4	0.29	0	6,6,6	0.21	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	4.63	1.45	1.22
3	A	1339	NO2	O1-N	4.55	1.45	1.22
3	E	1340	NO2	O1-N	4.48	1.44	1.22
3	F	1337	NO2	O1-N	4.46	1.44	1.22
3	B	1339	NO2	O1-N	4.45	1.44	1.22
3	F	1340	NO2	O1-N	4.43	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
4	A	1341	SO4	4	0
4	E	1343	SO4	1	0
3	B	1339	NO2	1	0
3	E	1340	NO2	1	0
4	C	1338	SO4	5	0
3	F	1337	NO2	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.31	4 (1%) 76 55	49, 66, 89, 112	1 (0%)
1	B	335/336 (99%)	-0.39	0 100 100	47, 66, 89, 112	0
1	C	334/336 (99%)	-0.42	1 (0%) 90 79	50, 66, 87, 113	1 (0%)
1	D	335/336 (99%)	-0.21	7 (2%) 63 40	29, 67, 88, 113	8 (2%)
1	E	335/336 (99%)	-0.39	2 (0%) 85 69	48, 65, 86, 110	1 (0%)
1	F	335/336 (99%)	-0.35	2 (0%) 85 69	49, 66, 89, 112	0
All	All	2009/2016 (99%)	-0.34	16 (0%) 82 64	29, 66, 89, 113	11 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136[A]	VAL	9.4
1	D	134[A]	GLY	9.3
1	E	5	LYS	4.9
1	D	135[A]	MET	4.6
1	D	133[A]	GLU	4.4
1	D	10	LYS	3.4
1	C	5	LYS	3.1
1	E	336	ARG	3.0
1	A	5	LYS	2.8
1	D	336	ARG	2.7
1	A	134	GLY	2.6
1	A	336	ARG	2.2
1	F	133	GLU	2.1
1	D	2	ASP	2.1
1	F	5	LYS	2.0
1	A	135	MET	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	SO4	E	1345	5/5	0.49	0.15	92,93,93,93	5
4	SO4	B	1343	5/5	0.59	0.16	78,78,79,79	5
4	SO4	E	1344	5/5	0.61	0.16	78,78,79,79	5
4	SO4	F	1341	5/5	0.74	0.20	72,73,73,74	5
4	SO4	A	1342	5/5	0.75	0.20	70,71,72,73	5
4	SO4	A	1343	5/5	0.78	0.16	74,74,75,75	5
4	SO4	C	1341	5/5	0.79	0.14	74,74,75,75	5
4	SO4	B	1342	5/5	0.80	0.13	76,77,77,78	5
4	SO4	B	1340	5/5	0.80	0.17	58,58,60,60	5
4	SO4	E	1342	5/5	0.81	0.20	67,67,67,68	5
4	SO4	D	1340	5/5	0.81	0.14	71,71,72,72	5
4	SO4	C	1340	5/5	0.86	0.12	63,64,64,64	5
4	SO4	D	1339	5/5	0.88	0.13	72,72,72,73	5
4	SO4	F	1342	5/5	0.89	0.14	67,67,68,68	5
4	SO4	C	1338	5/5	0.90	0.17	43,45,45,46	5
4	SO4	C	1339	5/5	0.91	0.10	60,61,62,62	5
4	SO4	E	1343	5/5	0.91	0.24	60,61,62,63	5
4	SO4	A	1340	5/5	0.92	0.10	71,71,71,72	5
4	SO4	E	1341	5/5	0.92	0.11	61,61,61,62	5
4	SO4	B	1341	5/5	0.93	0.10	62,63,63,63	5
4	SO4	A	1341	5/5	0.94	0.15	46,46,47,48	5
3	NO2	A	1339	3/3	0.98	0.08	63,63,64,64	0
2	CU	A	1337	1/1	0.99	0.04	77,77,77,77	1
3	NO2	B	1339	3/3	0.99	0.04	49,49,49,50	0
3	NO2	E	1337	3/3	0.99	0.06	68,68,68,68	0
3	NO2	E	1340	3/3	0.99	0.04	56,56,56,57	0
3	NO2	F	1337	3/3	0.99	0.06	58,58,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NO2	F	1340	3/3	0.99	0.06	72,72,73,73	0
2	CU	B	1337	1/1	0.99	0.06	66,66,66,66	1
2	CU	D	1337	1/1	0.99	0.04	85,85,85,85	1
2	CU	F	1338	1/1	0.99	0.05	116,116,116,116	0
2	CU	D	1338	1/1	1.00	0.01	58,58,58,58	0
2	CU	E	1338	1/1	1.00	0.03	49,49,49,49	1
2	CU	E	1339	1/1	1.00	0.01	57,57,57,57	0
2	CU	B	1338	1/1	1.00	0.01	55,55,55,55	0
2	CU	F	1339	1/1	1.00	0.01	54,54,54,54	0
2	CU	C	1336	1/1	1.00	0.04	65,65,65,65	1
2	CU	C	1337	1/1	1.00	0.01	60,60,60,60	0
2	CU	A	1338	1/1	1.00	0.01	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.