Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:26 PM GMT

PDB ID : 1AS8
Title : STRUCTURE OF NITRITE BOUND TO REDUCED ALCALIGENES FAE-
CALIS NITRITE REDUCTASE AT CRYO TEMPERATURE
Authors : Murphy, M.E.P.; Adman, E.T.; Turley, S.
Deposited on : 1997-08-13
Resolution : 1.85 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.85 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.
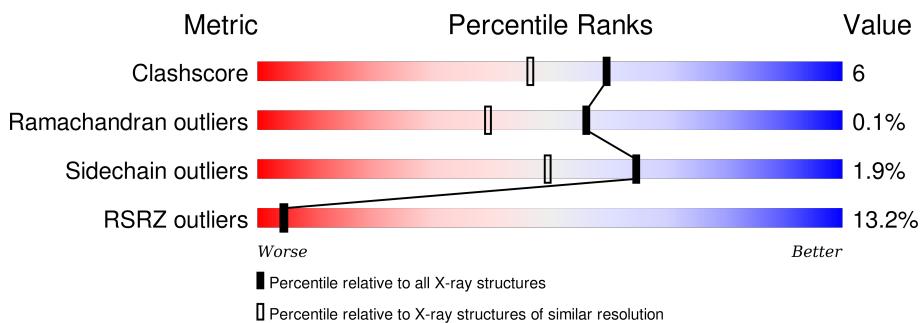
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	343	14% 82% 15% •
1	B	343	11% 85% 12% ••
1	C	343	14% 84% 13% ••
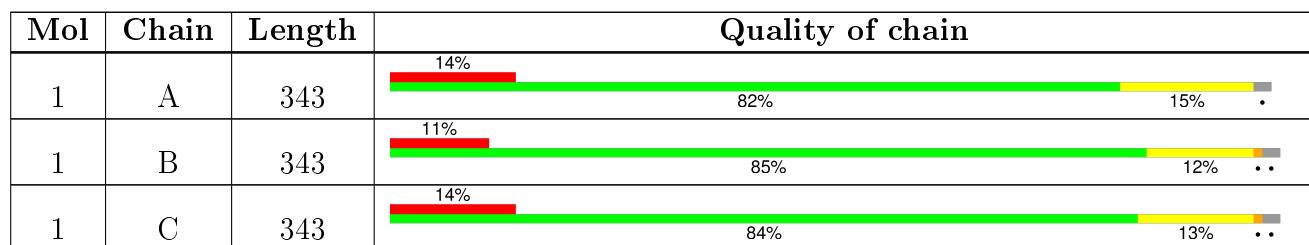
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NO2	A	503	-	-	-	X
3	NO2	B	503	-	-	X	X
3	NO2	C	503	-	-	X	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11412 atoms, of which 2994 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 NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	336	Total 3076	C 1639	H 516	N 430	O 480	S 11	0	0	0
1	B	336	Total 3076	C 1639	H 516	N 430	O 480	S 11	0	0	0
1	C	336	Total 3076	C 1639	H 516	N 430	O 480	S 11	0	0	0

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

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

- Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO_2).
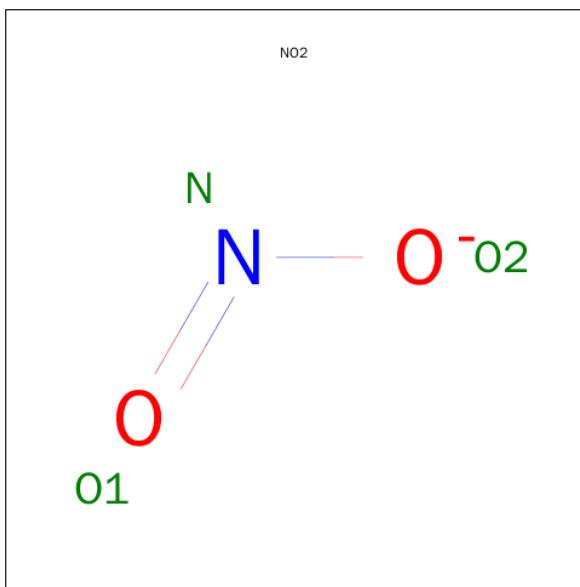
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total N O 3 1 2			0	0
3	B	1	Total N O 3 1 2			0	0
3	C	1	Total N O 3 1 2			0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	258	Total H O 774 516 258			0	0
4	B	231	Total H O 693 462 231			2	0
4	C	234	Total H O 702 468 234			0	0

3 Residue-property plots ⓘ

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

- Molecule 1: NITRITE REDUCTASE
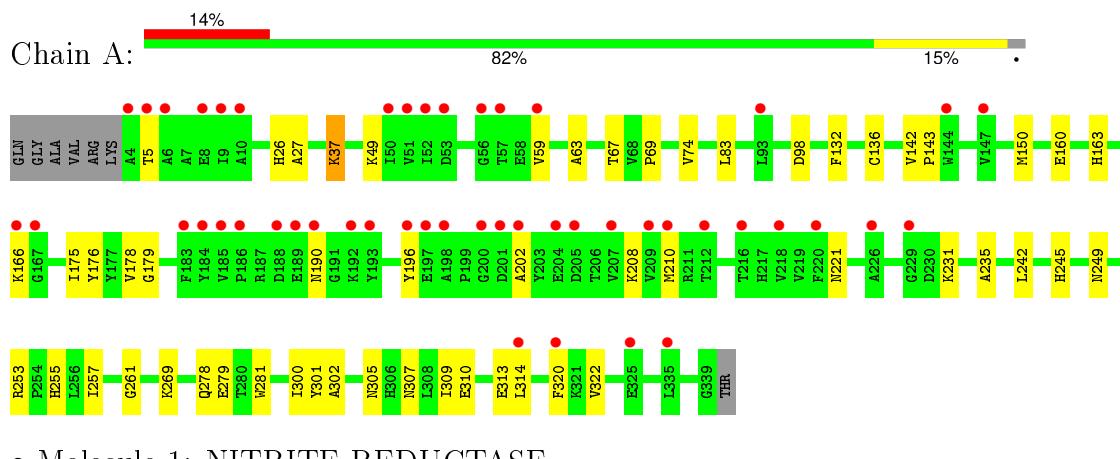
- Molecule 1: NITRITE REDUCTASE
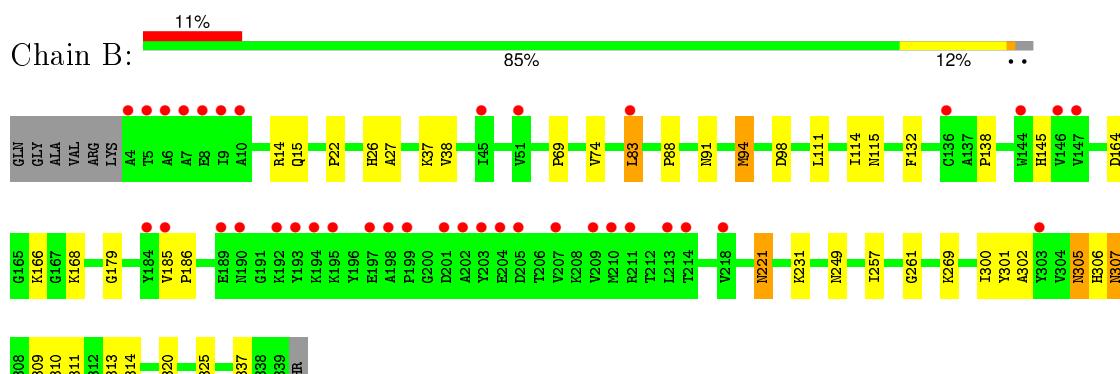
- Molecule 1: NITRITE REDUCTASE
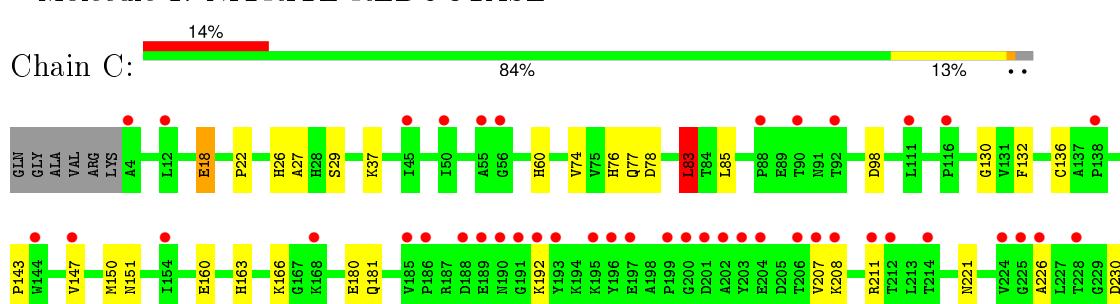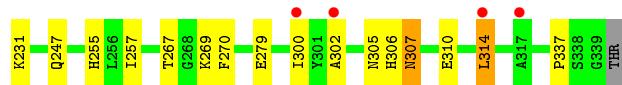
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.10Å 102.80Å 146.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.85 19.88 – 1.82	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.85) 71.2 (19.88-1.82)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.37 (at 1.82Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.194 , (Not available) 0.263 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	14.9	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.47$, $<L^2> = 0.31$	Xtriage
Outliers	0 of 59043 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	11412	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.52	0/2631	0.78	4/3588 (0.1%)
1	B	0.51	0/2631	0.77	5/3588 (0.1%)
1	C	0.51	0/2631	0.78	4/3588 (0.1%)
All	All	0.51	0/7893	0.78	13/10764 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	307	ASN	N-CA-C	-7.75	90.06	111.00
1	A	307	ASN	N-CA-C	-7.19	91.58	111.00
1	B	307	ASN	N-CA-C	-7.17	91.63	111.00
1	B	305	ASN	N-CA-C	-6.13	94.44	111.00
1	A	261	GLY	N-CA-C	-6.04	98.00	113.10
1	A	305	ASN	N-CA-C	-5.96	94.90	111.00
1	C	98	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	83	LEU	CA-CB-CG	5.62	128.24	115.30
1	C	305	ASN	N-CA-C	-5.59	95.90	111.00
1	C	83	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	98	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	98	ASP	CB-CG-OD2	5.28	123.06	118.30
1	B	261	GLY	N-CA-C	-5.20	100.10	113.10

There are no chirality outliers.

There are no planarity outliers.

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	2560	516	2485	29	8
1	B	2560	516	2485	27	5
1	C	2560	516	2485	34	2
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	3	0	0	1	0
3	B	3	0	0	2	0
3	C	3	0	0	2	0
4	A	258	516	0	1	13
4	B	231	462	0	1	6
4	C	234	468	0	2	9
All	All	8418	2994	7455	86	22

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 (86) 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:C:151:ASN:HD21	1:C:181:GLN:HE22	1.24	0.85
1:A:257:ILE:HG12	3:C:503:NO2:N	1.91	0.85
1:A:26:HIS:HE1	1:A:74:VAL:H	1.26	0.83
1:B:26:HIS:HE1	1:B:74:VAL:H	1.27	0.82
1:C:26:HIS:HE1	1:C:74:VAL:H	1.30	0.79
1:C:257:ILE:HD12	1:C:302:ALA:HB3	1.66	0.76
1:B:257:ILE:HD12	1:B:302:ALA:HB3	1.67	0.76
1:C:26:HIS:HD2	1:C:27:ALA:O	1.68	0.75
1:C:26:HIS:CE1	1:C:74:VAL:H	2.10	0.70
1:C:160:GLU:HG2	1:C:163:HIS:CE1	2.27	0.70
1:B:14:ARG:HG2	1:B:38:VAL:HB	1.74	0.67
3:A:503:NO2:N	1:B:257:ILE:HG12	2.09	0.67
1:B:26:HIS:CE1	1:B:74:VAL:H	2.10	0.67
1:A:136:CYS:HB2	1:A:150:MET:HG2	1.76	0.66
1:C:160:GLU:HG2	1:C:163:HIS:HE1	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:HD12	1:A:302:ALA:HB3	1.77	0.65
1:B:22:PRO:HB2	1:B:221:ASN:HD21	1.61	0.65
1:A:208:LYS:HD2	4:A:695:HOH:O	1.97	0.64
3:B:503:NO2:N	1:C:257:ILE:HG12	2.12	0.64
1:B:301:TYR:HB2	1:B:320:PHE:HB2	1.79	0.63
1:A:26:HIS:CE1	1:A:74:VAL:H	2.12	0.63
1:C:22:PRO:HB2	1:C:221:ASN:HD21	1.63	0.62
1:B:26:HIS:HD2	1:B:27:ALA:O	1.85	0.60
3:B:503:NO2:O2	1:C:257:ILE:HG12	2.02	0.60
1:B:132:PHE:CE1	1:B:269:LYS:HE3	2.38	0.58
1:B:310:GLU:HA	1:B:314:LEU:HB2	1.87	0.57
1:C:226:ALA:O	1:C:231:LYS:HB2	2.05	0.57
1:C:60:HIS:HD2	4:C:647:HOH:O	1.87	0.56
1:C:300:ILE:HD12	1:C:300:ILE:O	2.06	0.55
1:A:235:ALA:O	1:A:322:VAL:HA	2.08	0.53
1:C:255:HIS:ND1	1:C:279:GLU:O	2.42	0.53
1:A:26:HIS:HD2	1:A:27:ALA:O	1.92	0.53
1:C:22:PRO:HB2	1:C:221:ASN:ND2	2.24	0.52
1:C:310:GLU:HA	1:C:314:LEU:HB2	1.90	0.52
1:C:143:PRO:O	1:C:147:VAL:HG22	2.09	0.52
1:C:26:HIS:CD2	1:C:27:ALA:O	2.57	0.52
1:C:130:GLY:HA2	1:C:270:PHE:CD1	2.46	0.51
1:C:151:ASN:HD21	1:C:181:GLN:NE2	2.02	0.51
1:C:29:SER:O	1:C:76:HIS:CE1	2.64	0.50
1:A:37:LYS:N	1:A:37:LYS:HD3	2.26	0.50
1:A:249:ASN:O	1:B:307:ASN:HA	2.12	0.50
1:C:207:VAL:O	1:C:211:ARG:HG3	2.13	0.49
1:A:257:ILE:HG12	3:C:503:NO2:O2	2.13	0.48
1:A:310:GLU:HA	1:A:314:LEU:HB2	1.95	0.47
1:B:111:LEU:C	4:B:731:HOH:O	2.51	0.47
1:A:132:PHE:CE1	1:A:269:LYS:HE3	2.50	0.47
1:C:18:GLU:CD	1:C:18:GLU:H	2.17	0.47
1:A:196:TYR:CD2	1:A:202:ALA:HB2	2.50	0.47
1:B:88:PRO:HD2	1:B:91:ASN:ND2	2.30	0.46
1:A:309:ILE:O	1:A:313:GLU:HB2	2.15	0.46
1:B:69:PRO:HG3	1:B:179:GLY:HA3	1.97	0.46
1:A:142:VAL:HB	1:A:143:PRO:HD3	1.97	0.46
1:A:301:TYR:HB2	1:A:320:PHE:HB2	1.98	0.46
1:A:253:ARG:HA	1:A:281:TRP:O	2.16	0.46
1:C:136:CYS:HB2	1:C:150:MET:HG2	1.98	0.46
1:B:132:PHE:CD1	1:B:269:LYS:HE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:HIS:ND1	1:A:279:GLU:O	2.49	0.45
1:B:300:ILE:O	1:B:300:ILE:HG13	2.16	0.45
1:A:160:GLU:HG2	1:A:163:HIS:HE1	1.82	0.45
1:A:63:ALA:HB1	1:A:67:THR:O	2.17	0.45
1:A:166:LYS:O	1:A:166:LYS:HG2	2.15	0.45
1:C:130:GLY:HA2	1:C:270:PHE:CE1	2.52	0.44
1:A:278:GLN:OE1	1:C:267:THR:HB	2.16	0.44
1:B:15:GLN:HG3	1:B:15:GLN:O	2.17	0.44
1:C:77:GLN:O	1:C:78:ASP:HB2	2.17	0.44
1:B:185:VAL:HA	1:B:186:PRO:HD3	1.89	0.44
1:B:94:MET:HB2	1:B:115:ASN:ND2	2.33	0.43
1:C:208:LYS:HD3	1:C:208:LYS:HA	1.70	0.43
1:B:138:PRO:HG2	1:B:145:HIS:CE1	2.54	0.43
1:B:114:ILE:HG22	1:C:337:PRO:HB3	2.00	0.43
1:B:305:ASN:O	1:B:311:ALA:HB2	2.18	0.43
1:C:132:PHE:CE1	1:C:269:LYS:HE3	2.54	0.43
1:B:22:PRO:HB2	1:B:221:ASN:ND2	2.31	0.42
1:C:180:GLU:HB3	1:C:247:GLN:HG2	2.01	0.42
1:A:143:PRO:HB2	1:A:210:MET:HE1	2.02	0.42
1:A:69:PRO:HG3	1:A:179:GLY:HA3	2.02	0.42
1:B:249:ASN:O	1:C:307:ASN:HA	2.19	0.41
1:A:178:VAL:O	1:A:245:HIS:HA	2.21	0.41
1:C:143:PRO:HG2	4:C:560:HOH:O	2.21	0.41
1:A:49:LYS:HA	1:A:59:VAL:O	2.20	0.41
1:B:309:ILE:O	1:B:313:GLU:HB2	2.20	0.41
1:A:175:ILE:HA	1:A:242:LEU:O	2.21	0.41
1:C:83:LEU:HD13	1:C:85:LEU:HB2	2.03	0.41
1:A:160:GLU:HG2	1:A:163:HIS:CE1	2.57	0.40
1:B:164:ASP:OD2	1:B:168:LYS:HB3	2.22	0.40
1:B:306:HIS:ND1	1:B:306:HIS:O	2.54	0.40

All (22) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:555:HOH:O	4:B:568:HOH:H1[4_556]	1.19	0.41
4:A:651:HOH:O	4:C:530:HOH:O[3_645]	1.86	0.34
4:A:651:HOH:O	4:C:530:HOH:H1[3_645]	1.27	0.33
1:A:27:ALA:H	4:C:700:HOH:H2[3_645]	1.31	0.29
4:B:650:HOH:H1	4:B:719:HOH:O[4_556]	1.32	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLU:H	4:A:679:HOH:O[4_456]	1.41	0.19
1:A:5:THR:OG1	1:B:231:LYS:HZ3[4_456]	1.41	0.19
1:C:230:ASP:H	4:A:701:HOH:O[3_655]	1.43	0.17
1:A:176:TYR:OH	4:C:645:HOH:O[3_645]	2.08	0.12
4:A:606:HOH:O	4:C:599:HOH:H1[3_645]	1.51	0.09
1:A:5:THR:OG1	1:B:231:LYS:NZ[4_456]	2.12	0.08
4:A:555:HOH:O	4:B:568:HOH:O[4_556]	2.13	0.07
1:A:176:TYR:OH	4:C:645:HOH:H2[3_645]	1.54	0.06
4:A:563:HOH:O	4:B:601:HOH:O[4_556]	2.14	0.06
1:A:231:LYS:HZ3	1:C:226:ALA:O[3_645]	1.55	0.05
1:A:190:ASN:OD1	1:B:166:LYS:HZ3[1_655]	1.55	0.05
4:A:543:HOH:H2	4:B:603:HOH:O[4_556]	1.56	0.04
4:A:744:HOH:O	4:C:528:HOH:H2[3_645]	1.56	0.04
1:A:190:ASN:OD1	1:B:166:LYS:NZ[1_655]	2.16	0.04
4:A:518:HOH:O	4:C:537:HOH:O[3_645]	2.17	0.03
4:A:538:HOH:O	4:C:541:HOH:H1[3_645]	1.59	0.01
4:A:752:HOH:O	4:B:716:HOH:H1[4_556]	1.59	0.01

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	334/343 (97%)	326 (98%)	8 (2%)	0	100	100
1	B	334/343 (97%)	326 (98%)	8 (2%)	0	100	100
1	C	334/343 (97%)	327 (98%)	6 (2%)	1 (0%)	46	29
All	All	1002/1029 (97%)	979 (98%)	22 (2%)	1 (0%)	56	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	306	HIS

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	264/269 (98%)	260 (98%)	4 (2%)	72	60
1	B	264/269 (98%)	259 (98%)	5 (2%)	65	49
1	C	264/269 (98%)	258 (98%)	6 (2%)	58	41
All	All	792/807 (98%)	777 (98%)	15 (2%)	65	49

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	83	LEU
1	A	221	ASN
1	A	300	ILE
1	B	37	LYS
1	B	83	LEU
1	B	94	MET
1	B	221	ASN
1	B	337	PRO
1	C	18	GLU
1	C	37	LYS
1	C	83	LEU
1	C	166	LYS
1	C	192	LYS
1	C	314	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	77	GLN
1	A	163	HIS
1	A	221	ASN
1	A	296	GLN
1	B	15	GLN

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Mol	Chain	Res	Type
1	B	26	HIS
1	B	115	ASN
1	B	163	HIS
1	B	221	ASN
1	C	26	HIS
1	C	60	HIS
1	C	77	GLN
1	C	115	ASN
1	C	163	HIS
1	C	181	GLN
1	C	221	ASN

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 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	A	503	2	2,2,2	1.36	0	1,1,1	0.26	0
3	NO2	B	503	2	2,2,2	1.43	0	1,1,1	0.33	0
3	NO2	C	503	2	2,2,2	1.42	0	1,1,1	0.53	0

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In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NO2	A	503	2	-	0/0/0/0	0/0/0/0
3	NO2	B	503	2	-	0/0/0/0	0/0/0/0
3	NO2	C	503	2	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	NO2	1	0
3	B	503	NO2	2	0
3	C	503	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	336/343 (97%)	1.01	48 (14%)	4 3	7, 14, 36, 62	0
1	B	336/343 (97%)	0.83	38 (11%)	7 6	7, 15, 41, 70	0
1	C	336/343 (97%)	1.05	47 (13%)	4 3	8, 18, 38, 70	0
All	All	1008/1029 (97%)	0.96	133 (13%)	4 4	7, 15, 39, 70	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	189	GLU	6.1
1	C	192	LYS	5.1
1	A	10	ALA	5.1
1	B	6	ALA	5.0
1	A	190	ASN	4.8
1	B	4	ALA	4.4
1	A	189	GLU	4.3
1	A	5	THR	4.1
1	C	196	TYR	4.0
1	A	56	GLY	3.8
1	B	9	ILE	3.8
1	A	6	ALA	3.7
1	A	9	ILE	3.6
1	C	138	PRO	3.5
1	C	191	GLY	3.5
1	B	193	TYR	3.5
1	C	190	ASN	3.5
1	C	144	TRP	3.4
1	B	5	THR	3.3
1	B	7	ALA	3.3
1	C	201	ASP	3.3
1	A	144	TRP	3.2
1	C	56	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	192	LYS	3.2
1	C	186	PRO	3.2
1	B	10	ALA	3.2
1	C	204	GLU	3.2
1	A	204	GLU	3.1
1	C	203	TYR	3.1
1	A	325	GLU	3.1
1	B	192	LYS	3.1
1	B	195	LYS	3.1
1	A	51	VAL	3.1
1	C	188	ASP	3.1
1	A	188	ASP	3.1
1	B	204	GLU	3.0
1	A	59	VAL	3.0
1	A	218	VAL	2.9
1	A	183	PHE	2.9
1	B	202	ALA	2.9
1	C	50	ILE	2.8
1	A	209	VAL	2.8
1	C	212	THR	2.8
1	A	166	LYS	2.8
1	A	52	ILE	2.8
1	A	196	TYR	2.8
1	A	185	VAL	2.7
1	C	317	ALA	2.7
1	C	225	GLY	2.7
1	C	88	PRO	2.7
1	C	208	LYS	2.6
1	A	202	ALA	2.6
1	B	144	TRP	2.6
1	C	202	ALA	2.6
1	B	197	GLU	2.6
1	A	314	LEU	2.6
1	A	167	GLY	2.6
1	B	189	GLU	2.6
1	A	226	ALA	2.5
1	C	55	ALA	2.5
1	B	45	ILE	2.5
1	A	198	ALA	2.5
1	C	12	LEU	2.5
1	B	194	LYS	2.5
1	C	147	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	216	THR	2.5
1	B	199	PRO	2.5
1	C	185	VAL	2.5
1	C	207	VAL	2.5
1	B	51	VAL	2.4
1	B	203	TYR	2.4
1	B	83	LEU	2.4
1	B	213	LEU	2.4
1	A	220	PHE	2.4
1	C	228	THR	2.4
1	B	147	VAL	2.4
1	C	4	ALA	2.4
1	C	302	ALA	2.4
1	A	50	ILE	2.4
1	B	303	TYR	2.4
1	C	168	LYS	2.4
1	C	314	LEU	2.4
1	C	199	PRO	2.4
1	C	300	ILE	2.4
1	C	197	GLU	2.4
1	B	190	ASN	2.3
1	C	195	LYS	2.3
1	A	335	LEU	2.3
1	A	207	VAL	2.3
1	B	184	TYR	2.3
1	B	207	VAL	2.3
1	A	197	GLU	2.3
1	C	193	TYR	2.3
1	C	214	THR	2.3
1	C	226	ALA	2.3
1	A	184	TYR	2.3
1	B	8	GLU	2.2
1	A	4	ALA	2.2
1	B	146	VAL	2.2
1	C	206	THR	2.2
1	C	200	GLY	2.2
1	C	211	ARG	2.2
1	A	320	PHE	2.2
1	A	229	GLY	2.2
1	A	93	LEU	2.2
1	B	201	ASP	2.1
1	B	136	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	205	ASP	2.1
1	A	147	VAL	2.1
1	C	116	PRO	2.1
1	B	214	THR	2.1
1	C	92	THR	2.1
1	A	201	ASP	2.1
1	A	193	TYR	2.1
1	A	200	GLY	2.1
1	B	211	ARG	2.1
1	B	185	VAL	2.1
1	B	209	VAL	2.1
1	C	224	VAL	2.1
1	C	90	THR	2.1
1	A	8	GLU	2.1
1	A	186	PRO	2.1
1	C	111	LEU	2.1
1	B	218	VAL	2.1
1	B	205	ASP	2.1
1	A	210	MET	2.1
1	B	198	ALA	2.0
1	A	53	ASP	2.0
1	C	154	ILE	2.0
1	A	57	THR	2.0
1	A	212	THR	2.0
1	B	210	MET	2.0
1	C	45	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy
less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
3	NO2	A	503	3/3	0.61	0.37	13.22	16,16,16,16	3
3	NO2	B	503	3/3	0.78	0.44	12.34	26,26,29,29	3
3	NO2	C	503	3/3	0.70	0.44	10.67	26,26,26,28	3
2	CU	C	501	1/1	0.84	0.12	-1.60	19,19,19,19	0
2	CU	A	501	1/1	0.94	0.11	-2.07	17,17,17,17	0
2	CU	C	502	1/1	0.94	0.07	-3.13	16,16,16,16	0
2	CU	B	501	1/1	0.92	0.08	-5.53	19,19,19,19	0
2	CU	B	502	1/1	0.95	0.07	-	16,16,16,16	0
2	CU	A	502	1/1	0.92	0.09	-	14,14,14,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.