



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:43 PM UTC

PDB ID : 1AS8 / pdb_00001as8
Title : STRUCTURE OF NITRITE BOUND TO REDUCED ALCALIGENES FAECALIS 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)

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

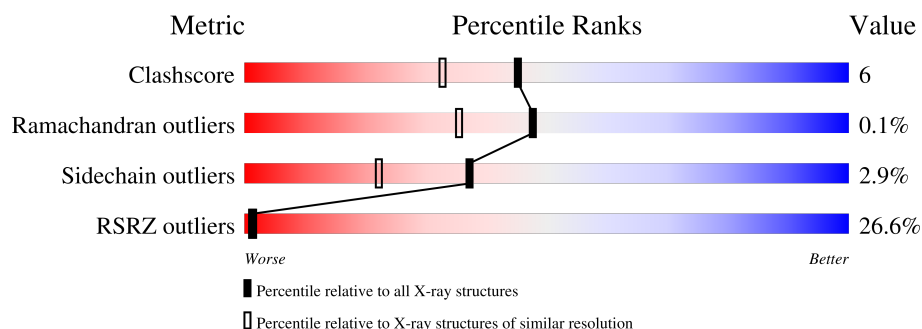
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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 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	343	27% 78% 19% ..
1	B	343	22% 81% 15% ...
1	C	343	29% 80% 16% ..

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	B	503	-	-	X	-
3	NO2	C	503	-	-	X	-

2 Entry composition

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.

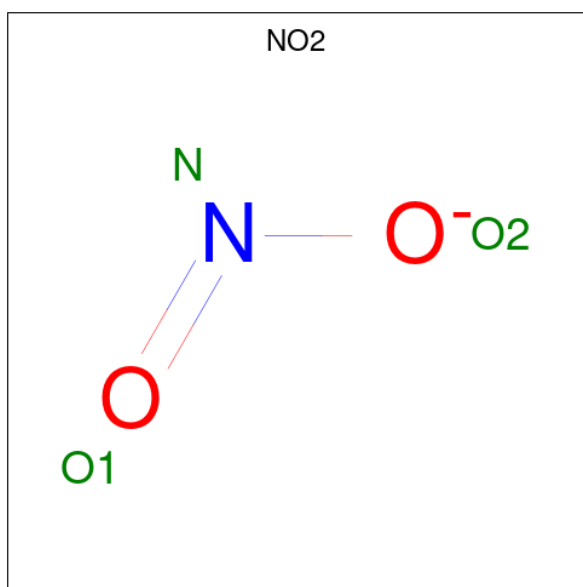
- Molecule 1 is a protein called NITRITE REDUCTASE.

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

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

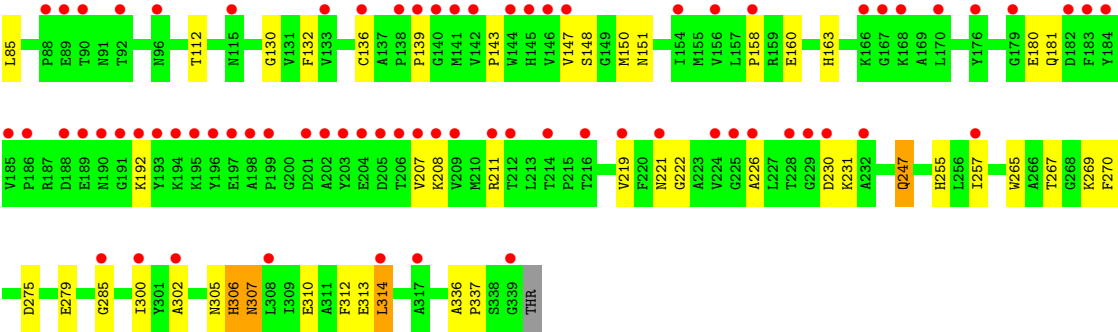
- Molecule 3 is NITRITE ION (CCD ID: NO2) (formula: NO₂).



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

- Molecule 4 is water.

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



4 Data and refinement statistics

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 10.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.85) 73.2 (10.00-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 1.82Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.194 , (Not available) 0.275 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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: 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	0.64	0/2631	1.08	19/3588 (0.5%)
1	B	0.63	1/2631 (0.0%)	1.08	17/3588 (0.5%)
1	C	0.63	0/2631	1.07	16/3588 (0.4%)
All	All	0.63	1/7893 (0.0%)	1.08	52/10764 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	MET	SD-CE	-5.55	1.65	1.79

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307	ASN	N-CA-C	-9.51	90.06	107.75
1	B	307	ASN	N-CA-C	-9.29	91.63	107.99
1	B	305	ASN	N-CA-C	-9.13	94.44	108.96
1	A	305	ASN	N-CA-C	-8.85	94.90	108.96
1	A	307	ASN	N-CA-C	-8.69	91.58	107.75
1	B	87	ASN	CA-C-N	8.37	128.43	119.89
1	B	87	ASN	C-N-CA	8.37	128.43	119.89
1	C	305	ASN	N-CA-C	-7.77	95.90	108.41
1	C	79	ASP	N-CA-C	-7.48	100.03	110.35
1	C	312	PHE	N-CA-C	7.46	122.56	113.38
1	A	79	ASP	N-CA-C	-7.45	100.92	110.53
1	B	185	VAL	N-CA-C	7.28	115.93	107.77
1	C	222	GLY	N-CA-C	7.18	124.88	115.40
1	C	63	ALA	N-CA-C	6.95	120.25	109.07
1	B	275	ASP	N-CA-C	-6.70	101.50	110.55
1	A	222	GLY	N-CA-C	6.41	123.86	115.40
1	A	261	GLY	N-CA-C	-6.40	98.00	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	PRO	N-CA-C	-6.23	101.48	111.38
1	B	306	HIS	N-CA-C	6.01	123.61	110.80
1	B	222	GLY	N-CA-C	5.96	123.28	115.36
1	C	306	HIS	N-CA-C	5.85	123.27	110.80
1	A	203	TYR	N-CA-C	5.79	118.09	111.02
1	A	275	ASP	N-CA-C	-5.77	102.77	110.55
1	B	79	ASP	N-CA-C	-5.74	102.27	110.59
1	A	87	ASN	CA-C-N	5.72	125.67	119.78
1	A	87	ASN	C-N-CA	5.72	125.67	119.78
1	A	219	VAL	N-CA-C	5.60	117.73	108.99
1	C	275	ASP	N-CA-C	-5.60	102.99	110.55
1	B	63	ALA	N-CA-C	5.58	118.20	108.76
1	A	63	ALA	N-CA-C	5.55	118.50	109.24
1	C	148	SER	N-CA-C	-5.54	106.41	112.72
1	B	261	GLY	N-CA-C	-5.52	100.10	113.18
1	B	303	TYR	N-CA-C	-5.51	99.54	108.52
1	C	313	GLU	N-CA-C	-5.50	106.61	113.55
1	A	309	ILE	N-CA-C	-5.44	105.22	110.72
1	C	285	GLY	N-CA-C	-5.34	105.11	111.36
1	B	148	SER	N-CA-C	-5.34	106.36	112.92
1	B	47	GLU	N-CA-C	-5.26	100.60	108.96
1	A	52	ILE	N-CA-C	5.21	117.90	112.90
1	B	52	ILE	N-CA-C	5.20	117.89	112.90
1	A	134	TYR	N-CA-C	-5.16	101.24	109.23
1	C	158	PRO	N-CA-C	-5.13	103.05	111.21
1	A	127	THR	N-CA-C	5.13	119.25	112.89
1	A	270	PHE	N-CA-C	5.12	118.79	112.54
1	A	185	VAL	N-CA-C	5.11	112.92	107.76
1	A	306	HIS	N-CA-C	5.10	121.66	110.80
1	B	311	ALA	N-CA-C	5.09	116.51	111.07
1	B	312	PHE	N-CA-C	5.06	119.60	113.38
1	C	265	TRP	N-CA-C	-5.05	99.77	108.56
1	C	47	GLU	N-CA-C	-5.02	100.97	108.96
1	C	219	VAL	N-CA-C	5.02	117.23	108.95
1	C	112	THR	N-CA-C	5.00	118.92	112.41

There are no chirality outliers.

There are no planarity outliers.

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	2560	516	2485	29	8
1	B	2560	516	2485	28	5
1	C	2560	516	2485	36	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	89	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 (89) 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:B:111:LEU:C	4:B:731:HOH:O	2.51	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:18:GLU:H	1:C:18:GLU:CD	2.17	0.51
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:A:132:PHE:CE1	1:A:269:LYS:HE3	2.50	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:253:ARG:HA	1:A:281:TRP:O	2.16	0.46
1:A:301:TYR:HB2	1:A:320:PHE:HB2	1.98	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:278:GLN:OE1	1:C:267:THR:HB	2.16	0.44
1:C:130:GLY:HA2	1:C:270:PHE:CE1	2.52	0.44
1:B:15:GLN:O	1:B:15:GLN:HG3	2.17	0.44
1:A:166:LYS:O	1:A:166:LYS:HG2	2.15	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:HA	1:C:208:LYS:HD3	1.70	0.43
1:B:114:ILE:HG22	1:C:337:PRO:HB3	2.00	0.43
1:B:138:PRO:HG2	1:B:145:HIS:CE1	2.54	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:26:HIS:CD2	1:C:26:HIS:C	2.97	0.42
1:C:180:GLU:HB3	1:C:247:GLN:HG2	2.01	0.42
1:A:69:PRO:HG3	1:A:179:GLY:HA3	2.02	0.42
1:C:336:ALA:O	1:C:337:PRO:C	2.62	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:A:49:LYS:HA	1:A:59:VAL:O	2.20	0.41
1:A:175:ILE:HA	1:A:242:LEU:O	2.21	0.41
1:B:309:ILE:O	1:B:313:GLU:HB2	2.20	0.41
1:C:83:LEU:HD13	1:C:85:LEU:HB2	2.03	0.41
1:C:143:PRO:HG2	4:C:560:HOH:O	2.21	0.41
1:A:160:GLU:HG2	1:A:163:HIS:CE1	2.57	0.40
1:B:58:GLU:CD	1:B:195:LYS:HE3	2.46	0.40
1:A:143:PRO:HB2	1:A:210:MET:HE1	2.03	0.40
1:B:164:ASP:OD2	1:B:168:LYS:HB3	2.22	0.40
1:B:306:HIS:O	1:B:306:HIS:ND1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:5:THR:OG1	1:B:231:LYS:HZ3[4_456]	1.41	0.19
1:B:325:GLU:H	4:A:679:HOH:O[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:190:ASN:OD1	1:B:166:LYS:HZ3[1_655]	1.55	0.05
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:NZ[1_655]	2.16	0.04
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
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	36	25
All	All	1002/1029 (97%)	979 (98%)	22 (2%)	1 (0%)	48	35

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%)	257 (97%)	7 (3%)	39	24
1	B	264/269 (98%)	255 (97%)	9 (3%)	32	17
1	C	264/269 (98%)	257 (97%)	7 (3%)	39	24
All	All	792/807 (98%)	769 (97%)	23 (3%)	37	22

All (23) 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	247	GLN
1	A	300	ILE
1	A	305	ASN
1	A	337	PRO
1	B	59	VAL
1	B	83	LEU
1	B	94	MET
1	B	204	GLU
1	B	221	ASN
1	B	247	GLN
1	B	305	ASN
1	B	314	LEU
1	B	337	PRO
1	C	18	GLU
1	C	37	LYS
1	C	83	LEU
1	C	139	PRO
1	C	192	LYS
1	C	247	GLN

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Mol	Chain	Res	Type
1	C	314	LEU

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

Mol	Chain	Res	Type
1	A	15	GLN
1	A	26	HIS
1	A	77	GLN
1	A	163	HIS
1	A	221	ASN
1	A	296	GLN
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	115	ASN
1	C	151	ASN
1	C	163	HIS
1	C	181	GLN
1	C	221	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1,2,2	4.15	1 (100%)	0,1,1	-	-
3	NO2	C	503	2	1,2,2	4.07	1 (100%)	0,1,1	-	-
3	NO2	B	503	2	1,2,2	4.28	1 (100%)	0,1,1	-	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	NO2	O1-N	4.28	1.43	1.22
3	A	503	NO2	O1-N	4.15	1.43	1.22
3	C	503	NO2	O1-N	4.07	1.42	1.22

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	C	503	NO2	2	0
3	B	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

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	336/343 (97%)	1.57	92 (27%)  	6, 12, 30, 62	0
1	B	336/343 (97%)	1.39	75 (22%)  	6, 13, 33, 67	0
1	C	336/343 (97%)	1.62	101 (30%)  	7, 15, 31, 63	0
All	All	1008/1029 (97%)	1.53	268 (26%)  	6, 13, 31, 67	0

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	ALA	8.0
1	B	4	ALA	6.5
1	B	6	ALA	6.5
1	C	192	LYS	6.0
1	C	189	GLU	5.7
1	B	9	ILE	5.6
1	A	10	ALA	5.4
1	A	191	GLY	5.3
1	C	196	TYR	5.3
1	C	188	ASP	5.2
1	A	188	ASP	5.2
1	B	204	GLU	5.1
1	A	190	ASN	5.0
1	C	208	LYS	4.9
1	A	6	ALA	4.9
1	C	138	PRO	4.9
1	A	229	GLY	4.8
1	B	5	THR	4.8
1	C	191	GLY	4.8
1	C	228	THR	4.8
1	A	189	GLU	4.7
1	A	56	GLY	4.7
1	B	193	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	207	VAL	4.5
1	A	192	LYS	4.5
1	C	168	LYS	4.5
1	B	203	TYR	4.5
1	A	4	ALA	4.5
1	C	201	ASP	4.4
1	C	203	TYR	4.4
1	B	7	ALA	4.4
1	C	207	VAL	4.3
1	C	204	GLU	4.3
1	A	8	GLU	4.2
1	A	5	THR	4.2
1	C	56	GLY	4.2
1	B	51	VAL	4.2
1	C	302	ALA	4.1
1	B	201	ASP	4.0
1	A	325	GLU	4.0
1	B	197	GLU	4.0
1	A	209	VAL	4.0
1	B	202	ALA	4.0
1	A	226	ALA	3.9
1	C	88	PRO	3.9
1	C	226	ALA	3.9
1	B	191	GLY	3.9
1	C	190	ASN	3.9
1	A	204	GLU	3.9
1	B	8	GLU	3.9
1	B	192	LYS	3.9
1	C	212	THR	3.9
1	B	11	ALA	3.7
1	A	196	TYR	3.7
1	C	147	VAL	3.6
1	B	144	TRP	3.6
1	B	195	LYS	3.6
1	B	198	ALA	3.6
1	B	189	GLU	3.6
1	A	7	ALA	3.5
1	A	205	ASP	3.5
1	C	90	THR	3.5
1	C	55	ALA	3.5
1	C	37	LYS	3.5
1	B	199	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	165	GLY	3.4
1	C	195	LYS	3.4
1	C	186	PRO	3.4
1	C	214	THR	3.4
1	A	167	GLY	3.3
1	A	52	ILE	3.3
1	B	209	VAL	3.3
1	C	202	ALA	3.3
1	B	214	THR	3.3
1	C	144	TRP	3.3
1	B	190	ASN	3.3
1	B	194	LYS	3.3
1	A	225	GLY	3.3
1	A	9	ILE	3.2
1	A	50	ILE	3.2
1	C	12	LEU	3.2
1	C	89	GLU	3.2
1	A	55	ALA	3.2
1	C	51	VAL	3.2
1	C	18	GLU	3.2
1	A	200	GLY	3.2
1	A	201	ASP	3.2
1	A	326	TRP	3.2
1	B	285	GLY	3.1
1	C	225	GLY	3.1
1	A	183	PHE	3.1
1	B	212	THR	3.1
1	A	202	ALA	3.1
1	A	207	VAL	3.1
1	A	198	ALA	3.1
1	B	211	ARG	3.0
1	B	56	GLY	3.0
1	B	336	ALA	3.0
1	C	317	ALA	3.0
1	A	193	TYR	3.0
1	A	148	SER	3.0
1	B	57	THR	3.0
1	A	53	ASP	3.0
1	A	214	THR	3.0
1	A	59	VAL	2.9
1	C	229	GLY	2.9
1	C	257	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	205	ASP	2.9
1	B	33	GLU	2.9
1	B	339	GLY	2.9
1	A	185	VAL	2.9
1	C	193	TYR	2.9
1	A	144	TRP	2.9
1	A	335	LEU	2.9
1	C	146	VAL	2.8
1	A	95	HIS	2.8
1	B	338	SER	2.8
1	B	45	ILE	2.8
1	C	50	ILE	2.8
1	C	64	PHE	2.8
1	A	140	GLY	2.8
1	B	200	GLY	2.8
1	C	22	PRO	2.8
1	C	211	ARG	2.8
1	C	199	PRO	2.8
1	A	166	LYS	2.7
1	C	8	GLU	2.7
1	B	196	TYR	2.7
1	C	179	GLY	2.7
1	A	186	PRO	2.7
1	A	89	GLU	2.7
1	A	147	VAL	2.7
1	C	209	VAL	2.7
1	A	311	ALA	2.7
1	B	55	ALA	2.7
1	C	339	GLY	2.7
1	B	136	CYS	2.7
1	A	57	THR	2.7
1	C	139	PRO	2.7
1	A	168	LYS	2.7
1	A	218	VAL	2.7
1	B	54	ASP	2.6
1	B	166	LYS	2.6
1	C	185	VAL	2.6
1	A	208	LYS	2.6
1	C	206	THR	2.6
1	A	220	PHE	2.6
1	C	69	PRO	2.6
1	A	314	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	300	ILE	2.6
1	A	66	GLY	2.6
1	C	53	ASP	2.6
1	C	63	ALA	2.6
1	C	224	VAL	2.6
1	C	197	GLU	2.6
1	C	16	LYS	2.6
1	A	212	THR	2.6
1	A	216	THR	2.6
1	B	93	LEU	2.5
1	C	194	LYS	2.5
1	A	51	VAL	2.5
1	A	184	TYR	2.5
1	B	230	ASP	2.5
1	C	230	ASP	2.5
1	A	197	GLU	2.5
1	C	57	THR	2.5
1	C	141	MET	2.5
1	C	205	ASP	2.5
1	C	167	GLY	2.5
1	C	170	LEU	2.5
1	B	121	ILE	2.5
1	B	300	ILE	2.5
1	A	27	ALA	2.5
1	C	32	ALA	2.5
1	C	92	THR	2.5
1	B	88	PRO	2.5
1	B	258	GLY	2.4
1	A	320	PHE	2.4
1	A	228	THR	2.4
1	C	54	ASP	2.4
1	C	182	ASP	2.4
1	A	224	VAL	2.4
1	A	145	HIS	2.4
1	B	184	TYR	2.4
1	B	213	LEU	2.4
1	C	48	LYS	2.4
1	C	58	GLU	2.4
1	C	96	ASN	2.4
1	C	221	ASN	2.4
1	A	210	MET	2.4
1	C	308	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	337	PRO	2.3
1	B	147	VAL	2.3
1	B	92	THR	2.3
1	C	176	TYR	2.3
1	B	115	ASN	2.3
1	C	4	ALA	2.3
1	C	158	PRO	2.3
1	C	83	LEU	2.3
1	B	220	PHE	2.3
1	C	232	ALA	2.3
1	B	187	ARG	2.3
1	B	12	LEU	2.3
1	C	314	LEU	2.3
1	C	140	GLY	2.2
1	C	184	TYR	2.2
1	C	115	ASN	2.2
1	B	141	MET	2.2
1	A	136	CYS	2.2
1	A	110	GLY	2.2
1	B	186	PRO	2.2
1	A	63	ALA	2.2
1	A	65	ASN	2.2
1	A	91	ASN	2.2
1	B	185	VAL	2.2
1	C	219	VAL	2.2
1	C	47	GLU	2.2
1	C	216	THR	2.2
1	C	285	GLY	2.2
1	A	143	PRO	2.2
1	C	13	PRO	2.2
1	B	183	PHE	2.2
1	B	283	ILE	2.2
1	C	25	VAL	2.2
1	C	133	VAL	2.2
1	A	29	SER	2.2
1	A	339	GLY	2.2
1	C	145	HIS	2.1
1	A	307	ASN	2.1
1	A	272	THR	2.1
1	B	68	VAL	2.1
1	C	156	VAL	2.1
1	C	136	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	199	PRO	2.1
1	A	263	TYR	2.1
1	B	188	ASP	2.1
1	A	142	VAL	2.1
1	B	210	MET	2.1
1	A	151	ASN	2.1
1	A	308	LEU	2.1
1	A	235	ALA	2.1
1	C	198	ALA	2.1
1	A	301	TYR	2.1
1	A	42	THR	2.1
1	B	37	LYS	2.1
1	C	166	LYS	2.1
1	A	334	VAL	2.1
1	C	59	VAL	2.1
1	A	139	PRO	2.1
1	B	143	PRO	2.1
1	B	314	LEU	2.1
1	B	89	GLU	2.0
1	B	165	GLY	2.0
1	B	22	PRO	2.0
1	C	17	VAL	2.0
1	C	142	VAL	2.0
1	C	72	LEU	2.0
1	A	11	ALA	2.0
1	B	49	LYS	2.0
1	A	255	HIS	2.0
1	A	309	ILE	2.0
1	C	60	HIS	2.0
1	C	154	ILE	2.0
1	C	183	PHE	2.0
1	A	117	GLY	2.0
1	B	228	THR	2.0
1	B	303	TYR	2.0
1	A	69	PRO	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 [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
3	NO2	A	503	3/3	0.42	0.21	16,16,16,16	3
3	NO2	B	503	3/3	0.62	0.24	26,26,29,29	3
2	CU	C	501	1/1	0.65	0.11	19,19,19,19	0
2	CU	B	501	1/1	0.71	0.11	19,19,19,19	0
2	CU	A	502	1/1	0.76	0.08	14,14,14,14	0
3	NO2	C	503	3/3	0.76	0.21	26,26,26,28	3
2	CU	B	502	1/1	0.78	0.09	16,16,16,16	0
2	CU	A	501	1/1	0.81	0.09	17,17,17,17	0
2	CU	C	502	1/1	0.84	0.06	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.