



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 04:43 PM BST

PDB ID : 5A2O
Title : Crystal structure of the nitrate transporter NRT1.1 from Arabidopsis thaliana in complex with nitrate.
Authors : Parker, J.L.; Newstead, S.
Deposited on : 2015-05-20
Resolution : 3.71 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

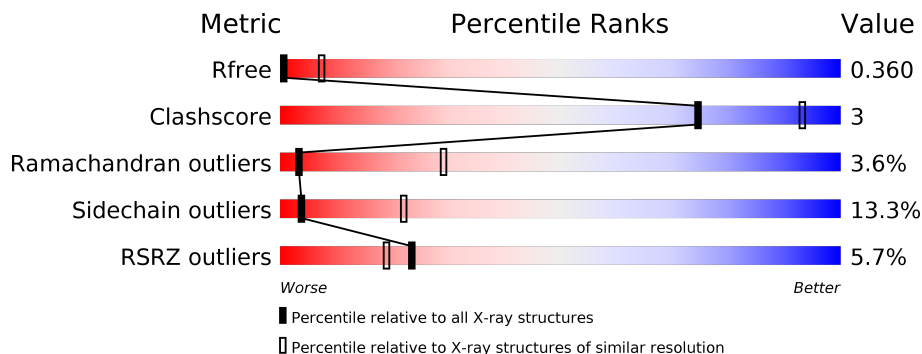
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	590	 3% 64% 14% • 20%
1	B	590	 6% 63% 15% • 20%

2 Entry composition [i](#)

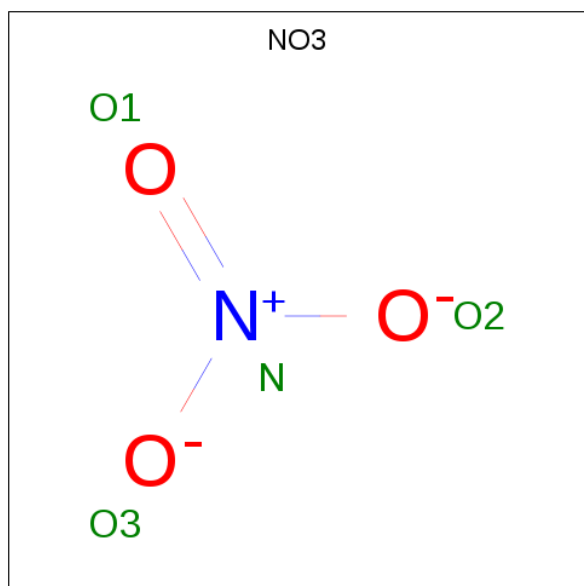
There are 2 unique types of molecules in this entry. The entry contains 13874 atoms, of which 6558 are hydrogens and 0 are deuteriums.

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 NITRATE TRANSPORTER 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	470	Total 6933	C 2408	H 3279	N 599	O 629	S 18	0	0	0
1	B	470	Total 6933	C 2408	H 3279	N 599	O 629	S 18	0	0	0

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO₃).

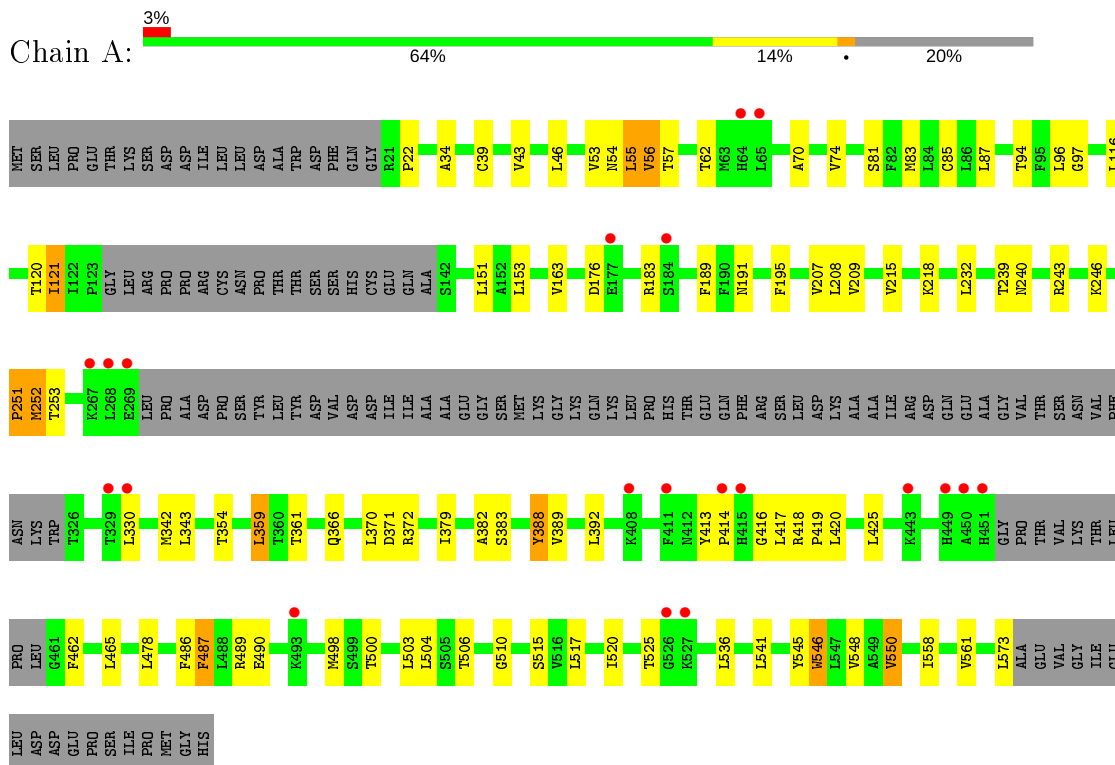


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	N O		
2	A	1	Total 4	N O 1 3	0	0
2	B	1	Total 4	N O 1 3	0	0

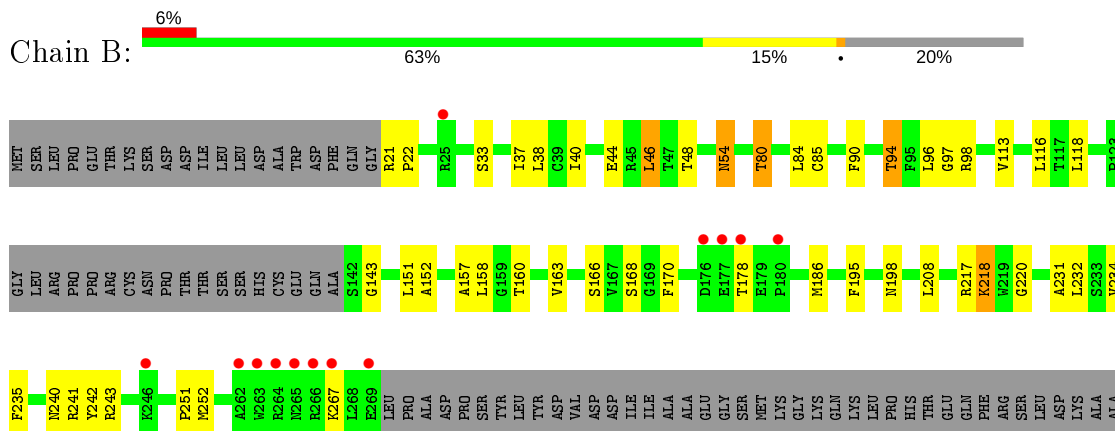
3 Residue-property plots

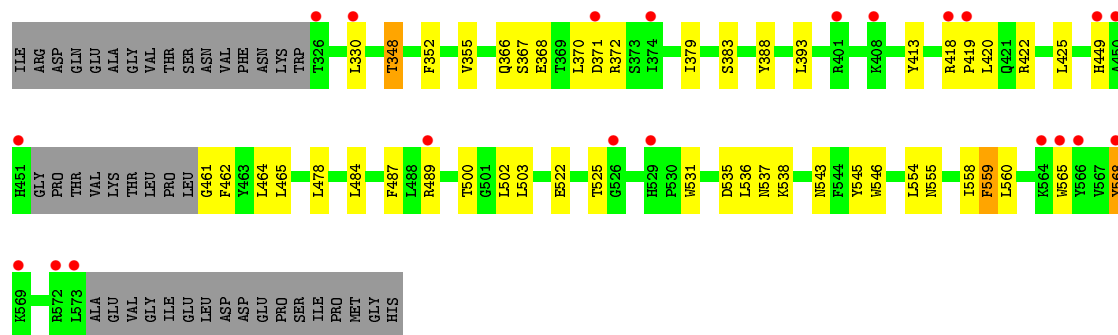
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NITRATE TRANSPORTER 1.1



- Molecule 1: NITRATE TRANSPORTER 1.1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.83Å 123.59Å 153.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.74 – 3.71 27.60 – 3.71	Depositor EDS
% Data completeness (in resolution range)	87.7 (27.74-3.71) 87.9 (27.60-3.71)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.74Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.287 , 0.328 0.316 , 0.360	Depositor DCC
R_{free} test set	1121 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	105.7	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 134.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.039 for k,h,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	13874	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: NO3

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	0.50	0/3734	0.66	0/5067
1	B	0.51	0/3734	0.67	0/5067
All	All	0.50	0/7468	0.66	0/10134

There are no bond length outliers.

There are no bond angle outliers.

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	3654	3279	3786	21	0
1	B	3654	3279	3786	27	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
All	All	7316	6558	7572	48	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:THR:HG23	1:B:84:LEU:HD23	1.66	0.77
1:A:56:VAL:HG22	1:A:74:VAL:HG21	1.69	0.73
1:B:80:THR:HG22	1:B:157:ALA:HB1	1.81	0.63
1:A:354:THR:HG22	1:A:510:GLY:O	2.00	0.61
1:A:388:TYR:CZ	1:A:392:LEU:HD11	2.36	0.61
1:A:39:CYS:O	1:A:43:VAL:HG23	2.05	0.56
1:B:37:ILE:HD13	1:B:170:PHE:CD2	2.40	0.56
1:B:535:ASP:HB3	1:B:538:LYS:HB2	1.89	0.54
1:B:151:LEU:HD23	1:B:152:ALA:N	2.23	0.52
1:B:352:PHE:O	1:B:355:VAL:HG22	2.10	0.52
1:A:388:TYR:CE1	1:A:392:LEU:HD11	2.44	0.52
1:B:348:THR:HG21	1:B:559:PHE:HB2	1.90	0.52
1:B:151:LEU:HD23	1:B:151:LEU:C	2.31	0.51
1:A:34:ALA:HB1	1:A:189:PHE:CE1	2.46	0.50
1:A:389:VAL:HA	1:A:392:LEU:HD12	1.93	0.49
1:A:55:LEU:HD11	1:A:153:LEU:HD22	1.95	0.49
1:B:217:ARG:O	1:B:220:GLY:N	2.45	0.49
1:A:209:VAL:HG11	1:A:382:ALA:HB3	1.95	0.48
1:A:70:ALA:O	1:A:74:VAL:HG23	2.14	0.48
1:A:546:TRP:HA	1:A:546:TRP:CE3	2.49	0.48
1:A:251:PRO:O	1:A:253:THR:N	2.47	0.47
1:A:546:TRP:HA	1:A:546:TRP:HE3	1.81	0.46
1:B:449:HIS:NE2	1:B:537:ASN:O	2.49	0.46
1:B:37:ILE:HD11	1:B:242:TYR:CD1	2.51	0.45
1:B:554:LEU:O	1:B:558:ILE:HG13	2.17	0.45
1:B:367:SER:O	1:B:372:ARG:NH1	2.50	0.45
1:B:90:PHE:O	1:B:94:THR:OG1	2.33	0.45
1:B:37:ILE:HD13	1:B:170:PHE:CE2	2.53	0.44
1:B:198:ASN:HB3	1:B:393:LEU:HD21	1.99	0.44
1:A:342:MET:HB2	1:A:487:PHE:CZ	2.53	0.44
1:A:120:THR:O	1:A:121:ILE:HG23	2.18	0.43
1:B:543:ASN:HA	1:B:546:TRP:HD1	1.82	0.43
1:B:231:ALA:HA	1:B:234:VAL:HG12	2.00	0.43
1:B:54:ASN:OD1	1:B:217:ARG:NH2	2.52	0.43
1:B:84:LEU:HD12	1:B:158:LEU:HD12	1.99	0.43
1:B:525:THR:HG21	1:B:531:TRP:CD1	2.54	0.43
1:A:359:LEU:HD11	1:A:388:TYR:HB2	2.01	0.43
1:A:546:TRP:O	1:A:550:VAL:HB	2.18	0.43
1:B:461:GLY:HA2	1:B:464:LEU:HD12	2.01	0.43
1:A:56:VAL:HG21	1:A:361:THR:HA	2.02	0.42
1:B:565:TRP:HA	1:B:568:TYR:HD1	1.84	0.42
1:B:80:THR:HG23	1:B:84:LEU:CD2	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HD11	1:B:235:PHE:CB	2.49	0.41
1:B:366:GLN:NE2	1:B:545:TYR:OH	2.53	0.41
1:A:486:PHE:O	1:A:490:GLU:N	2.53	0.41
1:A:517:LEU:HD23	1:A:548:VAL:HG22	2.02	0.41
1:A:366:GLN:NE2	1:A:545:TYR:OH	2.41	0.40
1:B:555:ASN:HA	1:B:558:ILE:HD12	2.02	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	462/590 (78%)	405 (88%)	39 (8%)	18 (4%)	3	27
1	B	462/590 (78%)	400 (87%)	47 (10%)	15 (3%)	4	31
All	All	924/1180 (78%)	805 (87%)	86 (9%)	33 (4%)	3	29

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	PRO
1	A	240	ASN
1	A	252	MET
1	A	413	TYR
1	A	414	PRO
1	B	22	PRO
1	B	252	MET
1	B	413	TYR
1	A	97	GLY
1	A	121	ILE
1	A	239	THR
1	A	371	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	419	PRO
1	B	96	LEU
1	B	97	GLY
1	B	143	GLY
1	B	166	SER
1	B	240	ASN
1	B	371	ASP
1	A	54	ASN
1	B	218	LYS
1	A	96	LEU
1	A	183	ARG
1	A	251	PRO
1	B	46	LEU
1	B	419	PRO
1	A	416	GLY
1	A	383	SER
1	A	418	ARG
1	B	54	ASN
1	B	418	ARG
1	A	215	VAL
1	B	251	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	386/489 (79%)	332 (86%)	54 (14%)	3	20
1	B	386/489 (79%)	337 (87%)	49 (13%)	4	23
All	All	772/978 (79%)	669 (87%)	103 (13%)	4	22

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	53	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	55	LEU
1	A	56	VAL
1	A	57	THR
1	A	62	THR
1	A	81	SER
1	A	83	MET
1	A	85	CYS
1	A	87	LEU
1	A	94	THR
1	A	116	LEU
1	A	151	LEU
1	A	163	VAL
1	A	176	ASP
1	A	191	ASN
1	A	195	PHE
1	A	207	VAL
1	A	208	LEU
1	A	218	LYS
1	A	232	LEU
1	A	243	ARG
1	A	246	LYS
1	A	252	MET
1	A	330	LEU
1	A	343	LEU
1	A	359	LEU
1	A	370	LEU
1	A	372	ARG
1	A	379	ILE
1	A	388	TYR
1	A	417	LEU
1	A	420	LEU
1	A	425	LEU
1	A	462	PHE
1	A	465	LEU
1	A	478	LEU
1	A	487	PHE
1	A	489	ARG
1	A	498	MET
1	A	500	THR
1	A	503	LEU
1	A	504	LEU
1	A	506	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	515	SER
1	A	520	ILE
1	A	525	THR
1	A	536	LEU
1	A	541	LEU
1	A	546	TRP
1	A	550	VAL
1	A	558	ILE
1	A	561	VAL
1	A	573	LEU
1	B	21	ARG
1	B	33	SER
1	B	38	LEU
1	B	44	GLU
1	B	46	LEU
1	B	48	THR
1	B	80	THR
1	B	85	CYS
1	B	94	THR
1	B	98	ARG
1	B	113	VAL
1	B	116	LEU
1	B	118	LEU
1	B	160	THR
1	B	163	VAL
1	B	168	SER
1	B	178	THR
1	B	186	MET
1	B	195	PHE
1	B	208	LEU
1	B	218	LYS
1	B	232	LEU
1	B	241	ARG
1	B	243	ARG
1	B	267	LYS
1	B	330	LEU
1	B	348	THR
1	B	368	GLU
1	B	370	LEU
1	B	379	ILE
1	B	383	SER
1	B	388	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	420	LEU
1	B	422	ARG
1	B	425	LEU
1	B	462	PHE
1	B	465	LEU
1	B	478	LEU
1	B	484	LEU
1	B	487	PHE
1	B	489	ARG
1	B	500	THR
1	B	502	LEU
1	B	503	LEU
1	B	522	GLU
1	B	536	LEU
1	B	559	PHE
1	B	560	LEU
1	B	568	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	240	ASN
1	A	555	ASN
1	B	72	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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
2	NO3	B	1574	-	1,3,3	0.17	0	0,3,3	0.00	-
2	NO3	A	1574	-	1,3,3	0.42	0	0,3,3	0.00	-

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.

No monomer is involved in short contacts.

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	470/590 (79%)	-0.05	20 (4%) 35 29	5, 91, 271, 300	0
1	B	470/590 (79%)	0.09	34 (7%) 15 12	3, 86, 234, 299	0
All	All	940/1180 (79%)	0.02	54 (5%) 23 19	3, 88, 245, 300	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	LEU	5.9
1	B	569	LYS	5.7
1	B	371	ASP	5.5
1	B	573	LEU	5.0
1	B	568	TYR	4.9
1	A	443	LYS	4.7
1	A	414	PRO	4.5
1	B	269	GLU	4.3
1	A	329	THR	4.3
1	B	326	THR	4.2
1	A	269	GLU	4.0
1	A	449	HIS	3.9
1	A	527	LYS	3.9
1	A	450	ALA	3.8
1	A	415	HIS	3.6
1	B	451	HIS	3.5
1	B	401	ARG	3.5
1	A	267	LYS	3.4
1	B	267	LYS	3.4
1	B	565	TRP	3.4
1	B	265	ASN	3.2
1	B	264	ARG	3.1
1	B	572	ARG	3.1
1	B	177	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	564	LYS	2.9
1	B	180	PRO	2.9
1	B	408	LYS	2.9
1	B	450	ALA	2.9
1	A	177	GLU	2.8
1	A	64	HIS	2.8
1	B	25	ARG	2.7
1	A	268	LEU	2.6
1	A	184	SER	2.6
1	A	65	LEU	2.5
1	B	529	HIS	2.5
1	A	411	PHE	2.5
1	B	418	ARG	2.5
1	A	493	LYS	2.5
1	A	526	GLY	2.4
1	B	449	HIS	2.4
1	A	451	HIS	2.4
1	B	526	GLY	2.4
1	B	419	PRO	2.4
1	B	246	LYS	2.3
1	B	330	LEU	2.3
1	B	374	ILE	2.2
1	B	263	TRP	2.1
1	B	176	ASP	2.1
1	B	489	ARG	2.1
1	B	266	ARG	2.1
1	B	178	THR	2.1
1	B	566	TYR	2.0
1	A	408	LYS	2.0
1	B	262	ALA	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 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, 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(\AA^2)	Q<0.9
2	NO3	B	1574	4/4	0.81	0.55	64,68,68,70	0
2	NO3	A	1574	4/4	0.81	0.67	64,68,68,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.