



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:26 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

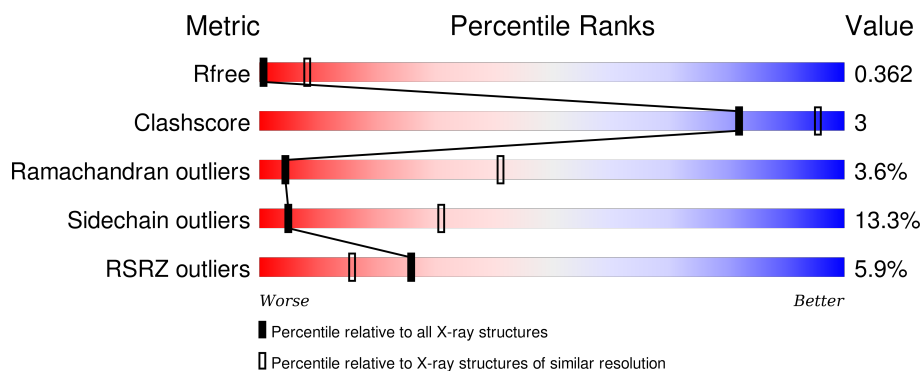
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1129 (3.94-3.50)
Clashscore	102246	1252 (3.94-3.50)
Ramachandran outliers	100387	1199 (3.94-3.50)
Sidechain outliers	100360	1197 (3.94-3.50)
RSRZ outliers	91569	1136 (3.94-3.50)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>3%</div> <div>64%</div> <div>14%</div> <div>•</div> <div>20%</div> </div>
1	B	590	<div> <div>6%</div> <div>63%</div> <div>15%</div> <div>•</div> <div>20%</div> </div>

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
2	NO3	A	1574	-	-	-	X
2	NO3	B	1574	-	-	-	X

## 2 Entry composition [i](#)

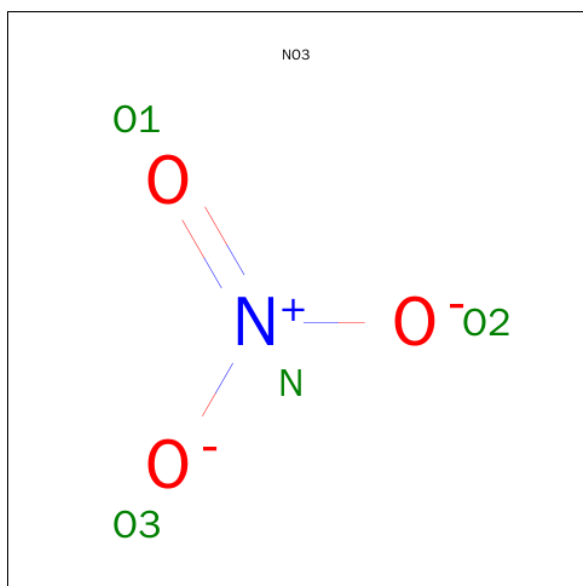
There are 2 unique types of molecules in this entry. The entry contains 13874 atoms, of which 6558 are hydrogens and 0 are deuteriums.

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.

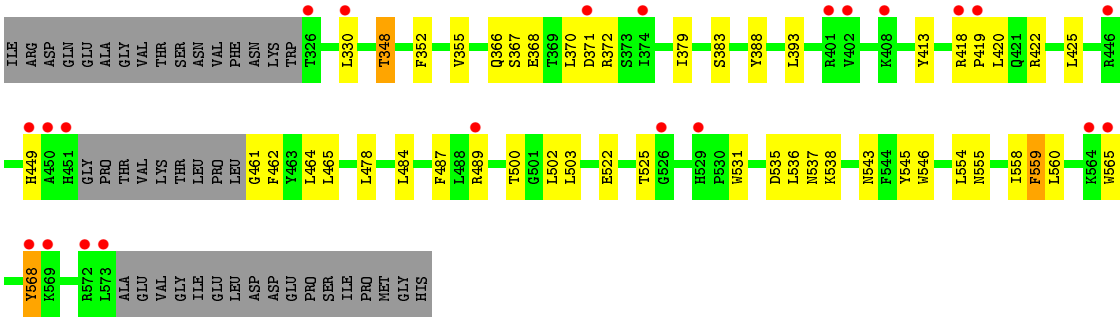
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	470	Total	C	H	N	O	S	0	0	0
			6933	2408	3279	599	629	18			
1	B	470	Total	C	H	N	O	S	0	0	0
			6933	2408	3279	599	629	18			

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 3.74Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.287 , 0.328 0.312 , 0.362	Depositor DCC
$R_{free}$ test set	1119 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	105.7	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 135.0	EDS
Estimated twinning fraction	0.039 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 22013 reflections	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	13874	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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

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:54:ASN:OD1	1:B:217:ARG:NH2	2.52	0.43
1:B:231:ALA:HA	1:B:234:VAL:HG12	2.00	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

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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%)	4	38
1	B	462/590 (78%)	400 (87%)	47 (10%)	15 (3%)	5	44
All	All	924/1180 (78%)	805 (87%)	86 (9%)	33 (4%)	4	41

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

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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 ⓘ

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%)	4	29
1	B	386/489 (79%)	337 (87%)	49 (13%)	5	32
All	All	772/978 (79%)	669 (87%)	103 (13%)	5	31

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

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

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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

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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

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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 ⓘ

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

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	A	1574	-	1,3,3	0.53	0	0,3,3	0.00	-
2	NO3	B	1574	-	1,3,3	0.11	0	0,3,3	0.00	-

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
2	NO3	A	1574	-	-	0/0/0/0	0/0/0/0
2	NO3	B	1574	-	-	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.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	470/590 (79%)	-0.04	20 (4%)	39	26	5, 91, 271, 300	0
1	B	470/590 (79%)	0.11	35 (7%)	17	11	3, 86, 234, 299	0
All	All	940/1180 (79%)	0.04	55 (5%)	26	16	3, 88, 245, 300	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	LEU	6.1
1	B	371	ASP	5.7
1	B	569	LYS	5.6
1	B	568	TYR	5.3
1	B	573	LEU	5.0
1	A	414	PRO	4.8
1	A	443	LYS	4.6
1	B	326	THR	4.3
1	A	329	THR	4.3
1	B	269	GLU	4.2
1	A	269	GLU	4.1
1	A	449	HIS	4.0
1	A	415	HIS	4.0
1	A	527	LYS	3.9
1	B	401	ARG	3.7
1	B	451	HIS	3.7
1	A	450	ALA	3.6
1	A	267	LYS	3.4
1	B	267	LYS	3.4
1	B	565	TRP	3.3
1	B	265	ASN	3.2
1	B	572	ARG	3.2
1	B	264	ARG	3.1
1	B	177	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	450	ALA	3.0
1	B	564	LYS	2.9
1	A	177	GLU	2.9
1	B	408	LYS	2.8
1	B	529	HIS	2.8
1	B	180	PRO	2.8
1	A	184	SER	2.7
1	A	411	PHE	2.7
1	A	493	LYS	2.6
1	A	64	HIS	2.6
1	B	526	GLY	2.5
1	B	418	ARG	2.5
1	B	449	HIS	2.5
1	A	268	LEU	2.5
1	B	25	ARG	2.5
1	B	176	ASP	2.4
1	B	489	ARG	2.4
1	B	374	ILE	2.4
1	A	526	GLY	2.4
1	B	330	LEU	2.3
1	A	65	LEU	2.3
1	A	451	HIS	2.3
1	B	419	PRO	2.3
1	B	246	LYS	2.3
1	B	263	TRP	2.3
1	B	266	ARG	2.1
1	B	178	THR	2.1
1	B	446	ARG	2.1
1	A	572	ARG	2.0
1	B	262	ALA	2.0
1	B	402	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	NO3	B	1574	4/4	0.80	0.57	9.63	64,68,68,70	0
2	NO3	A	1574	4/4	0.81	0.68	6.45	64,68,68,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.