



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:43 PM UTC

PDB ID : 5A2O / pdb_00005a2o
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 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

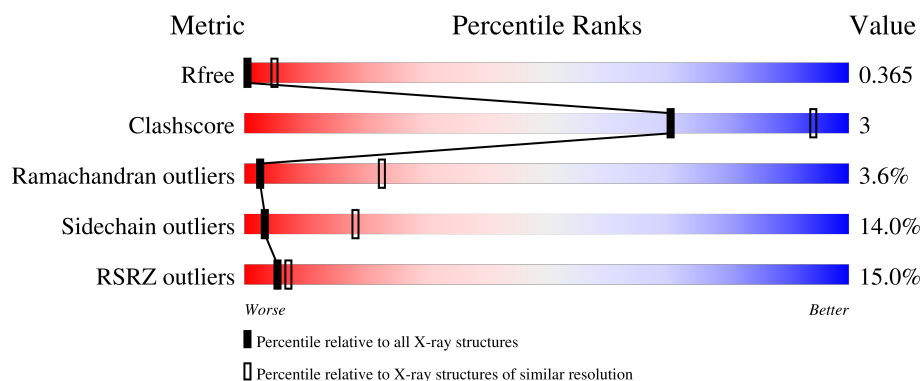
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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}	180053	1182 (3.84-3.60)
Clashscore	190562	1222 (3.84-3.60)
Ramachandran outliers	187476	1178 (3.84-3.60)
Sidechain outliers	187428	1174 (3.84-3.60)
RSRZ outliers	180081	1181 (3.84-3.60)

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	590	12% 62% 16% • 20%
1	B	590	12% 61% 16% • 20%

2 Entry composition [i](#)

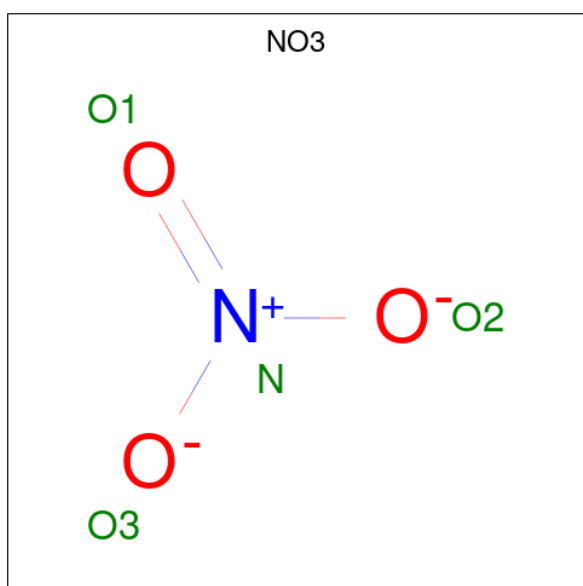
There are 2 unique types of molecules in this entry. The entry contains 13874 atoms, of which 6558 are hydrogens and 0 are deuteriums.

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
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 (CCD ID: NO3) (formula: NO₃).

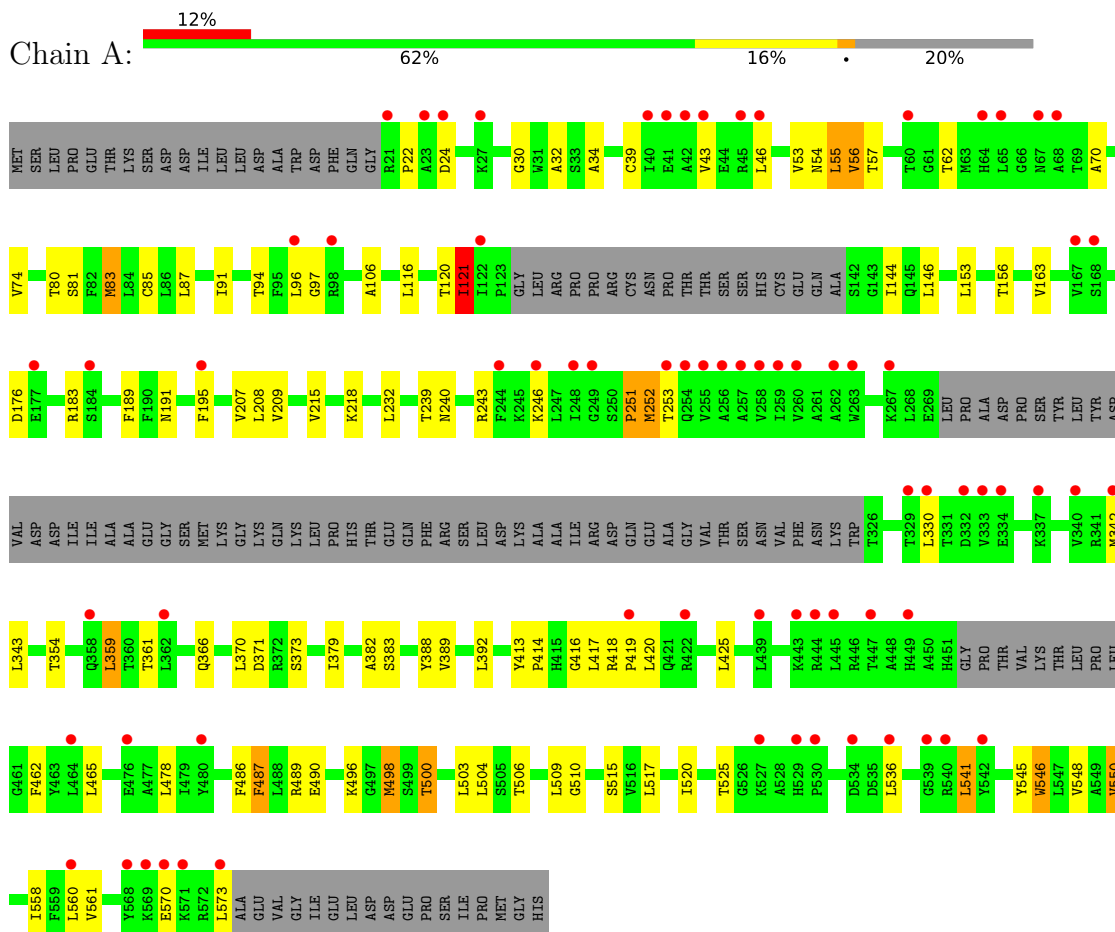


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		

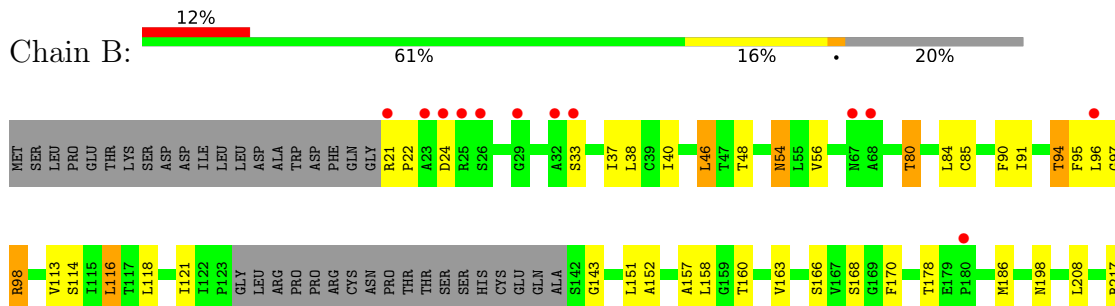
3 Residue-property plots

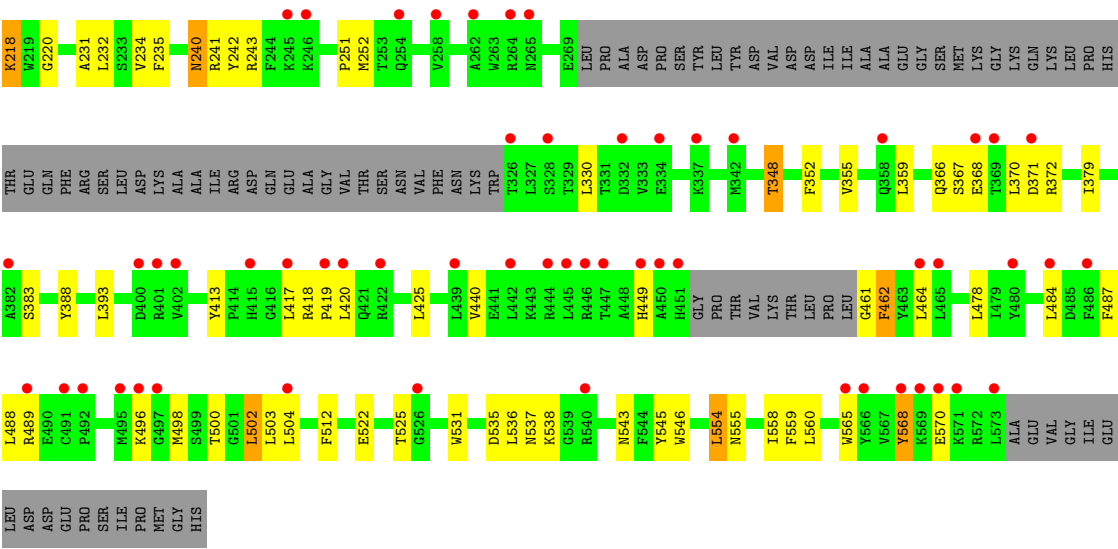
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 27.74 – 3.71	Depositor EDS
% Data completeness (in resolution range)	87.7 (27.74-3.71) 87.6 (27.74-3.71)	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 0.318 , 0.365	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 , 125.6	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 ⓘ

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	0.86	0/3734	1.24	10/5067 (0.2%)
1	B	0.87	0/3734	1.28	14/5067 (0.3%)
All	All	0.87	0/7468	1.26	24/10134 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ASN	CA-CB-CG	7.81	120.41	112.60
1	A	500	THR	N-CA-C	-6.99	104.57	113.23
1	A	30	GLY	N-CA-C	6.83	120.69	111.20
1	A	541	LEU	N-CA-C	6.62	118.50	111.28
1	B	121	ILE	N-CA-C	6.29	122.43	109.34
1	B	56	VAL	N-CA-C	-6.24	104.43	110.42
1	B	98	ARG	N-CA-C	-6.23	104.40	112.68
1	A	498	MET	N-CA-C	-5.94	105.85	112.57
1	B	462	PHE	CA-CB-CG	5.89	119.69	113.80
1	A	106	ALA	N-CA-C	-5.86	104.25	111.40
1	B	116	LEU	N-CA-C	-5.67	105.18	111.36
1	B	512	PHE	CA-CB-CG	5.55	119.36	113.80
1	B	498	MET	N-CA-C	-5.50	106.45	112.72
1	A	373	SER	N-CA-C	5.40	117.86	110.24
1	B	554	LEU	CA-C-N	5.34	127.69	120.38
1	B	554	LEU	C-N-CA	5.34	127.69	120.38
1	B	95	PHE	N-CA-C	5.33	117.18	108.55
1	B	24	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	146	LEU	N-CA-C	-5.23	105.66	111.36
1	A	156	THR	N-CA-C	-5.17	105.73	111.36
1	A	24	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	32	ALA	N-CA-C	-5.07	105.75	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	502	LEU	N-CA-C	-5.05	105.86	111.36
1	B	488	LEU	N-CA-C	-5.03	105.51	111.69

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	22	0
1	B	3654	3279	3786	29	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
All	All	7316	6558	7572	51	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 (51) 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:A:83:MET:HE1	1:A:509:LEU:HD11	1.87	0.56
1:B:151:LEU:HD23	1:B:151:LEU:C	2.31	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:217:ARG:O	1:B:218:LYS:C	2.62	0.42
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:352:PHE:CD1	1:B:352:PHE:C	2.98	0.42
1:B:80:THR:HG23	1:B:84:LEU:CD2	2.45	0.41
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

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	462/590 (78%)	405 (88%)	39 (8%)	18 (4%)	2	21
1	B	462/590 (78%)	400 (87%)	47 (10%)	15 (3%)	3	25
All	All	924/1180 (78%)	805 (87%)	86 (9%)	33 (4%)	2	23

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
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

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Mol	Chain	Res	Type
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%)	328 (85%)	58 (15%)	3	16
1	B	386/489 (79%)	336 (87%)	50 (13%)	4	20
All	All	772/978 (79%)	664 (86%)	108 (14%)	3	18

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	53	VAL
1	A	55	LEU
1	A	56	VAL
1	A	57	THR
1	A	62	THR
1	A	80	THR
1	A	81	SER
1	A	83	MET
1	A	85	CYS
1	A	87	LEU
1	A	91	ILE
1	A	94	THR
1	A	116	LEU
1	A	121	ILE

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Mol	Chain	Res	Type
1	A	144	ILE
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	379	ILE
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	496	LYS
1	A	498	MET
1	A	500	THR
1	A	503	LEU
1	A	504	LEU
1	A	506	THR
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	560	LEU
1	A	561	VAL
1	A	570	GLU

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Mol	Chain	Res	Type
1	A	573	LEU
1	B	21	ARG
1	B	33	SER
1	B	38	LEU
1	B	46	LEU
1	B	48	THR
1	B	80	THR
1	B	85	CYS
1	B	91	ILE
1	B	94	THR
1	B	98	ARG
1	B	113	VAL
1	B	114	SER
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	208	LEU
1	B	232	LEU
1	B	241	ARG
1	B	243	ARG
1	B	330	LEU
1	B	348	THR
1	B	359	LEU
1	B	368	GLU
1	B	370	LEU
1	B	379	ILE
1	B	383	SER
1	B	388	TYR
1	B	417	LEU
1	B	420	LEU
1	B	425	LEU
1	B	440	VAL
1	B	462	PHE
1	B	478	LEU
1	B	484	LEU
1	B	487	PHE
1	B	489	ARG
1	B	496	LYS

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Mol	Chain	Res	Type
1	B	500	THR
1	B	502	LEU
1	B	503	LEU
1	B	504	LEU
1	B	522	GLU
1	B	536	LEU
1	B	560	LEU
1	B	568	TYR
1	B	570	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	212	GLN
1	A	366	GLN
1	A	412	ASN
1	A	468	GLN
1	A	543	ASN
1	A	555	ASN
1	B	412	ASN
1	B	415	HIS
1	B	421	GLN

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](#)

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	0.45	0	0,3,3	-	-
2	NO3	B	1574	-	1,3,3	0.21	0	0,3,3	-	-

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%)	0.74	73 (15%)  	5, 90, 271, 300	0
1	B	470/590 (79%)	0.70	68 (14%)  	3, 87, 235, 299	0
All	All	940/1180 (79%)	0.72	141 (15%)  	3, 89, 245, 300	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	VAL	6.6
1	B	566	TYR	5.8
1	A	329	THR	5.8
1	A	330	LEU	5.4
1	A	334	GLU	5.4
1	A	333	VAL	5.2
1	B	371	ASP	5.1
1	B	486	PHE	5.1
1	A	464	LEU	5.0
1	B	25	ARG	4.9
1	B	419	PRO	4.8
1	A	67	ASN	4.8
1	B	21	ARG	4.8
1	A	256	ALA	4.7
1	A	443	LYS	4.6
1	B	450	ALA	4.6
1	B	180	PRO	4.3
1	B	491	CYS	4.3
1	B	420	LEU	4.2
1	A	255	VAL	4.0
1	A	342	MET	4.0
1	B	342	MET	3.9
1	B	258	VAL	3.8
1	A	573	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	257	ALA	3.7
1	A	27	LYS	3.6
1	B	444	ARG	3.6
1	A	449	HIS	3.6
1	B	382	ALA	3.5
1	B	24	ASP	3.5
1	B	29	GLY	3.5
1	B	569	LYS	3.5
1	A	246	LYS	3.5
1	A	24	ASP	3.4
1	B	246	LYS	3.3
1	B	445	LEU	3.3
1	B	422	ARG	3.2
1	A	444	ARG	3.2
1	A	184	SER	3.2
1	A	254	GLN	3.2
1	A	536	LEU	3.2
1	B	264	ARG	3.1
1	B	33	SER	3.1
1	A	540	ARG	3.1
1	B	484	LEU	3.1
1	A	569	LYS	3.1
1	A	445	LEU	3.0
1	A	96	LEU	3.0
1	A	439	LEU	3.0
1	A	340	VAL	3.0
1	B	23	ALA	3.0
1	A	262	ALA	3.0
1	A	177	GLU	2.9
1	B	568	TYR	2.9
1	A	476	GLU	2.9
1	B	495	MET	2.9
1	B	540	ARG	2.9
1	A	362	LEU	2.9
1	A	45	ARG	2.9
1	B	451	HIS	2.9
1	B	489	ARG	2.9
1	B	337	LYS	2.9
1	B	526	GLY	2.8
1	B	442	LEU	2.8
1	B	492	PRO	2.8
1	A	337	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	464	LEU	2.8
1	B	262	ALA	2.8
1	A	422	ARG	2.8
1	B	67	ASN	2.8
1	B	265	ASN	2.8
1	A	244	PHE	2.8
1	A	260	VAL	2.7
1	B	480	TYR	2.7
1	A	570	GLU	2.7
1	B	497	GLY	2.7
1	A	21	ARG	2.7
1	B	496	LYS	2.7
1	A	41	GLU	2.7
1	B	32	ALA	2.7
1	B	449	HIS	2.6
1	A	358	GLN	2.6
1	A	571	LYS	2.6
1	A	534	ASP	2.6
1	A	248	ILE	2.6
1	B	565	TRP	2.6
1	A	46	LEU	2.6
1	A	122	ILE	2.6
1	A	40	ILE	2.5
1	A	65	LEU	2.5
1	A	542	TYR	2.5
1	A	447	THR	2.5
1	B	447	THR	2.5
1	B	401	ARG	2.5
1	A	332	ASP	2.5
1	A	267	LYS	2.5
1	A	529	HIS	2.4
1	B	326	THR	2.4
1	B	465	LEU	2.4
1	B	504	LEU	2.4
1	B	358	GLN	2.4
1	A	195	PHE	2.4
1	A	568	TYR	2.4
1	A	560	LEU	2.4
1	A	98	ARG	2.4
1	B	439	LEU	2.4
1	B	400	ASP	2.4
1	A	480	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	334	GLU	2.4
1	A	168	SER	2.3
1	A	253	THR	2.3
1	B	96	LEU	2.3
1	B	254	GLN	2.3
1	A	539	GLY	2.3
1	B	571	LYS	2.2
1	A	419	PRO	2.2
1	B	68	ALA	2.2
1	B	368	GLU	2.2
1	B	328	SER	2.2
1	B	402	VAL	2.2
1	B	573	LEU	2.2
1	A	530	PRO	2.2
1	A	68	ALA	2.2
1	B	332	ASP	2.2
1	A	167	VAL	2.1
1	A	527	LYS	2.1
1	A	23	ALA	2.1
1	B	417	LEU	2.1
1	A	259	ILE	2.1
1	A	43	VAL	2.1
1	A	60	THR	2.1
1	B	245	LYS	2.1
1	A	42	ALA	2.1
1	B	415	HIS	2.0
1	A	263	TRP	2.0
1	B	446	ARG	2.0
1	B	26	SER	2.0
1	A	249	GLY	2.0
1	A	64	HIS	2.0
1	B	369	THR	2.0
1	B	570	GLU	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
2	NO3	B	1574	4/4	0.94	0.14	64,68,68,70	0
2	NO3	A	1574	4/4	0.97	0.12	64,68,68,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.