



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:33 PM UTC

PDB ID : 5A2N / pdb_00005a2n
Title : Crystal structure of the nitrate transporter NRT1.1 from Arabidopsis thaliana.
Authors : Parker, J.L.; Newstead, S.
Deposited on : 2015-05-20
Resolution : 3.70 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
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

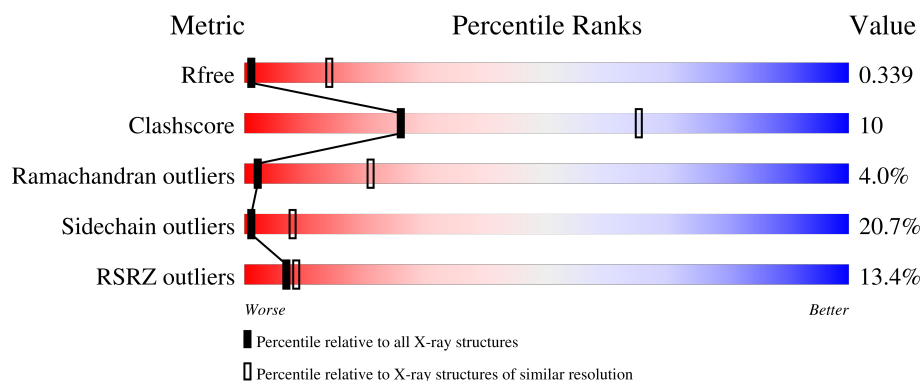
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	11% 49% 24% 6% 20%
1	B	590	10% 48% 23% 7% 20%

2 Entry composition

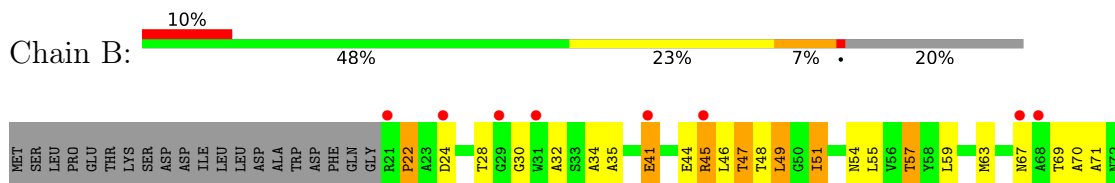
There is only 1 type of molecule in this entry. The entry contains 7474 atoms, of which 166 are hydrogens and 0 are deuteriums.

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 PROTEIN NRT1/ PTR FAMILY 6.3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	470	Total	C	H	N	O	S	0	0	0
			3737	2408	83	599	629	18			
1	B	470	Total	C	H	N	O	S	0	0	0
			3737	2408	83	599	629	18			

- Molecule 1: PROTEIN NRT1/ PTR FAMILY 6.3





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.80Å 124.03Å 153.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.53 – 3.70 27.53 – 3.70	Depositor EDS
% Data completeness (in resolution range)	86.3 (27.53-3.70) 86.0 (27.53-3.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.74Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.278 , 0.310 0.307 , 0.339	Depositor DCC
R_{free} test set	1105 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	105.4	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 85.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	7474	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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 ⓘ

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	2/3734 (0.1%)	1.57	46/5067 (0.9%)
1	B	0.88	2/3734 (0.1%)	1.61	57/5067 (1.1%)
All	All	0.87	4/7468 (0.1%)	1.59	103/10134 (1.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	MET	SD-CE	6.63	1.96	1.79
1	A	122	ILE	CA-C	5.53	1.58	1.52
1	A	466	ILE	CA-CB	5.19	1.57	1.53
1	B	266	ARG	CA-C	5.15	1.59	1.52

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	498	MET	N-CA-C	-9.60	99.40	112.94
1	A	500	THR	N-CA-C	-8.86	102.46	113.18
1	B	24	ASP	CA-CB-CG	7.88	120.48	112.60
1	A	95	PHE	N-CA-C	7.49	120.63	108.34
1	A	24	ASP	CA-CB-CG	7.45	120.05	112.60
1	A	97	GLY	CA-C-N	7.24	134.44	121.92
1	A	97	GLY	C-N-CA	7.24	134.44	121.92
1	A	32	ALA	N-CA-C	-7.01	103.65	111.71
1	B	95	PHE	CA-C-N	7.01	134.92	121.54
1	B	95	PHE	C-N-CA	7.01	134.92	121.54
1	A	421	GLN	CA-C-N	6.89	129.51	120.28
1	A	421	GLN	C-N-CA	6.89	129.51	120.28
1	A	207	VAL	N-CA-C	6.85	117.64	110.72
1	B	499	SER	N-CA-C	-6.84	105.07	113.41
1	B	49	LEU	CA-C-N	6.72	127.58	119.99
1	B	49	LEU	C-N-CA	6.72	127.58	119.99
1	A	498	MET	N-CA-C	-6.63	102.47	111.55
1	A	192	ARG	N-CA-C	-6.60	104.85	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	PHE	N-CA-C	6.52	120.09	109.59
1	A	185	LYS	CA-C-N	6.42	129.12	120.65
1	A	185	LYS	C-N-CA	6.42	129.12	120.65
1	A	196	CYS	N-CA-C	-6.40	105.36	113.43
1	B	370	LEU	N-CA-C	6.31	119.52	110.24
1	A	23	ALA	N-CA-C	6.19	116.18	108.19
1	B	155	LEU	N-CA-C	-6.18	105.88	113.41
1	B	35	ALA	CA-C-N	6.16	128.44	120.44
1	B	35	ALA	C-N-CA	6.16	128.44	120.44
1	B	264	ARG	N-CA-C	-6.10	105.67	113.23
1	A	466	ILE	N-CA-CB	6.07	114.33	110.50
1	A	122	ILE	N-CA-C	6.04	121.92	108.88
1	B	257	ALA	CA-C-N	6.01	128.95	120.42
1	B	257	ALA	C-N-CA	6.01	128.95	120.42
1	A	541	LEU	N-CA-C	5.99	117.61	111.14
1	B	348	THR	CA-C-N	5.99	128.62	120.54
1	B	348	THR	C-N-CA	5.99	128.62	120.54
1	B	488	LEU	N-CA-C	-5.93	104.16	111.40
1	B	122	ILE	N-CA-C	5.92	121.68	108.88
1	A	247	LEU	CA-C-N	5.86	131.15	123.06
1	A	247	LEU	C-N-CA	5.86	131.15	123.06
1	B	498	MET	CA-C-N	5.83	132.53	122.09
1	B	498	MET	C-N-CA	5.83	132.53	122.09
1	B	178	THR	N-CA-C	-5.76	105.91	113.17
1	A	465	LEU	CA-C-N	5.72	123.84	120.24
1	A	465	LEU	C-N-CA	5.72	123.84	120.24
1	B	240	ASN	CA-CB-CG	5.67	118.27	112.60
1	B	156	THR	N-CA-C	-5.66	105.48	112.90
1	B	208	LEU	N-CA-C	5.59	118.14	111.71
1	A	55	LEU	CA-C-N	5.56	127.56	120.56
1	A	55	LEU	C-N-CA	5.56	127.56	120.56
1	B	372	ARG	N-CA-C	5.50	122.52	110.80
1	A	156	THR	N-CA-C	-5.50	105.44	111.82
1	A	97	GLY	N-CA-C	5.46	122.22	112.22
1	B	166	SER	N-CA-C	5.46	120.32	113.43
1	B	370	LEU	CA-C-N	5.46	131.97	121.54
1	B	370	LEU	C-N-CA	5.46	131.97	121.54
1	B	554	LEU	CA-C-N	5.46	127.60	120.28
1	B	554	LEU	C-N-CA	5.46	127.60	120.28
1	B	110	ALA	CA-C-N	5.45	127.85	120.44
1	B	110	ALA	C-N-CA	5.45	127.85	120.44
1	B	444	ARG	N-CA-C	-5.44	106.31	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	THR	CA-C-N	5.42	127.59	120.60
1	B	73	THR	C-N-CA	5.42	127.59	120.60
1	A	38	LEU	N-CA-C	5.42	119.00	112.38
1	B	171	GLY	CA-C-N	5.40	127.52	120.28
1	B	171	GLY	C-N-CA	5.40	127.52	120.28
1	A	373	SER	N-CA-C	5.37	117.81	110.24
1	B	176	ASP	N-CA-C	5.37	116.80	109.18
1	B	497	GLY	CA-C-N	5.35	130.60	122.37
1	B	497	GLY	C-N-CA	5.35	130.60	122.37
1	B	258	VAL	N-CA-C	-5.34	105.32	110.72
1	A	247	LEU	N-CA-C	5.30	117.25	109.24
1	A	251	PRO	CA-C-N	5.30	131.66	121.54
1	A	251	PRO	C-N-CA	5.30	131.66	121.54
1	A	105	PHE	N-CA-C	5.27	119.58	113.20
1	B	44	GLU	CA-C-N	5.25	127.31	120.28
1	B	44	GLU	C-N-CA	5.25	127.31	120.28
1	B	247	LEU	CA-C-N	5.24	128.92	122.37
1	B	247	LEU	C-N-CA	5.24	128.92	122.37
1	A	111	THR	CA-C-N	5.23	125.90	119.99
1	A	111	THR	C-N-CA	5.23	125.90	119.99
1	B	171	GLY	N-CA-C	-5.22	106.03	113.86
1	A	106	ALA	N-CA-C	-5.21	104.54	112.04
1	B	233	SER	CA-C-N	5.20	127.30	120.60
1	B	233	SER	C-N-CA	5.20	127.30	120.60
1	B	30	GLY	CA-C-N	5.14	127.89	120.38
1	B	30	GLY	C-N-CA	5.14	127.89	120.38
1	B	202	LEU	CA-C-N	5.14	127.17	120.28
1	B	202	LEU	C-N-CA	5.14	127.17	120.28
1	B	482	GLY	CA-C-N	5.14	127.43	120.38
1	B	482	GLY	C-N-CA	5.14	127.43	120.38
1	A	358	GLN	CA-C-N	5.13	127.57	120.29
1	A	358	GLN	C-N-CA	5.13	127.57	120.29
1	A	32	ALA	CA-C-N	5.10	127.43	120.54
1	A	32	ALA	C-N-CA	5.10	127.43	120.54
1	B	98	ARG	N-CA-C	-5.09	107.02	113.18
1	A	95	PHE	CA-C-N	5.08	129.63	122.46
1	A	95	PHE	C-N-CA	5.08	129.63	122.46
1	A	372	ARG	CA-C-N	5.05	128.02	120.90
1	A	372	ARG	C-N-CA	5.05	128.02	120.90
1	A	111	THR	N-CA-C	-5.05	105.24	111.40
1	A	345	ILE	N-CA-C	-5.04	105.79	110.53
1	B	70	ALA	N-CA-C	-5.03	107.27	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	487	PHE	N-CA-C	5.03	118.90	112.87

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	83	3786	68	0
1	B	3654	83	3786	74	0
All	All	7308	166	7572	142	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 10.

All (142) 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:263:TRP:HA	1:B:266:ARG:HB3	1.67	0.76
1:B:250:SER:HB2	1:B:251:PRO:HA	1.67	0.75
1:B:251:PRO:O	1:B:254:GLN:HG3	1.87	0.74
1:A:108:ILE:HG21	1:A:158:LEU:HD23	1.68	0.73
1:B:57:THR:HB	1:B:217:ARG:HH22	1.56	0.71
1:A:56:VAL:HG22	1:A:74:VAL:HG21	1.72	0.70
1:B:327:LEU:HA	1:B:330:LEU:HB2	1.72	0.70
1:A:250:SER:HB2	1:A:251:PRO:HA	1.74	0.70
1:A:93:ASP:HB3	1:A:249:GLY:HA3	1.74	0.69
1:B:243:ARG:HG3	1:B:245:LYS:HE3	1.75	0.68
1:A:440:VAL:HB	1:A:444:ARG:HH21	1.57	0.68
1:B:425:LEU:HB3	1:B:478:LEU:HD23	1.76	0.68
1:B:32:ALA:HB1	1:B:241:ARG:HE	1.61	0.66
1:A:418:ARG:HA	1:A:422:ARG:HD3	1.78	0.65
1:A:425:LEU:HB3	1:A:478:LEU:HD23	1.78	0.65
1:B:479:ILE:HG12	1:B:483:GLN:HE21	1.61	0.64
1:A:96:LEU:O	1:A:100:LEU:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:TRP:HB2	1:B:264:ARG:NH1	2.15	0.61
1:A:142:SER:HA	1:A:145:GLN:HB2	1.82	0.61
1:A:77:PHE:CE1	1:A:157:ALA:HB2	2.35	0.61
1:A:115:ILE:HG22	1:A:152:ALA:HB2	1.83	0.60
1:B:251:PRO:HD3	1:B:498:MET:HB3	1.83	0.59
1:A:56:VAL:HG21	1:A:361:THR:HA	1.85	0.59
1:A:240:ASN:C	1:A:242:TYR:H	2.11	0.59
1:B:440:VAL:HG12	1:B:444:ARG:HE	1.68	0.59
1:B:32:ALA:HB1	1:B:241:ARG:NE	2.18	0.58
1:A:54:ASN:O	1:A:56:VAL:N	2.37	0.58
1:A:479:ILE:HG12	1:A:483:GLN:HE21	1.69	0.58
1:A:32:ALA:HB3	1:A:241:ARG:HB2	1.86	0.57
1:B:118:LEU:HA	1:B:121:ILE:HG12	1.87	0.56
1:B:243:ARG:HG3	1:B:245:LYS:CE	2.34	0.56
1:B:67:ASN:HB2	1:B:534:ASP:HA	1.88	0.56
1:A:342:MET:HB2	1:A:487:PHE:CE1	2.41	0.55
1:B:151:LEU:HG	1:B:155:LEU:HD12	1.89	0.55
1:A:45:ARG:HH11	1:A:45:ARG:HA	1.72	0.55
1:B:351:LEU:HB3	1:B:552:VAL:HG22	1.89	0.55
1:B:201:SER:O	1:B:205:VAL:HG23	2.06	0.55
1:B:362:LEU:HD22	1:B:541:LEU:HD11	1.89	0.55
1:B:217:ARG:HG2	1:B:221:TYR:CE2	2.42	0.54
1:B:263:TRP:HB2	1:B:264:ARG:CZ	2.38	0.53
1:B:342:MET:HG2	1:B:346:TRP:HB2	1.91	0.53
1:B:359:LEU:HD11	1:B:469:TYR:HA	1.91	0.53
1:B:45:ARG:HA	1:B:45:ARG:NH1	2.23	0.53
1:B:251:PRO:HD2	1:B:252:MET:HG2	1.91	0.52
1:B:182:GLU:O	1:B:186:MET:HB2	2.09	0.52
1:A:44:GLU:OE1	1:A:164:LYS:HG3	2.10	0.51
1:A:345:ILE:O	1:A:348:THR:HG22	2.09	0.51
1:B:205:VAL:HG21	1:B:389:VAL:HG21	1.92	0.51
1:A:247:LEU:HG	1:A:248:ILE:N	2.26	0.51
1:B:445:LEU:C	1:B:447:THR:H	2.19	0.50
1:A:37:ILE:HG13	1:A:242:TYR:CZ	2.46	0.50
1:A:429:PHE:HA	1:A:432:MET:HB2	1.93	0.50
1:B:109:GLN:HB3	1:B:159:GLY:HA3	1.94	0.50
1:B:54:ASN:HD22	1:B:382:ALA:HB3	1.76	0.50
1:B:265:ASN:HA	1:B:268:LEU:HB2	1.93	0.50
1:A:438:ALA:HB2	1:A:545:TYR:CB	2.41	0.49
1:A:77:PHE:HA	1:A:154:TYR:CE2	2.46	0.49
1:A:501:GLY:C	1:A:503:LEU:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:PRO:HD3	1:A:498:MET:HB3	1.94	0.49
1:B:34:ALA:HB1	1:B:189:PHE:CE2	2.48	0.49
1:B:85:CYS:HA	1:B:161:GLY:O	2.13	0.49
1:B:420:LEU:HA	1:B:423:ILE:HD12	1.95	0.49
1:A:32:ALA:CB	1:A:241:ARG:HB2	2.43	0.48
1:A:250:SER:HB2	1:A:251:PRO:CA	2.42	0.48
1:B:212:GLN:HG2	1:B:217:ARG:HG3	1.95	0.48
1:B:59:LEU:HA	1:B:63:MET:HB3	1.94	0.48
1:A:174:GLN:HB2	1:A:186:MET:HE3	1.95	0.48
1:B:260:VAL:C	1:B:262:ALA:H	2.22	0.48
1:B:254:GLN:HE22	1:B:495:MET:HE1	1.79	0.48
1:A:356:HIS:O	1:A:359:LEU:HB3	2.14	0.48
1:A:413:TYR:CB	1:A:414:PRO:HD3	2.44	0.47
1:A:243:ARG:HA	1:A:243:ARG:HD2	1.56	0.47
1:B:54:ASN:HD22	1:B:382:ALA:CB	2.27	0.47
1:B:442:LEU:HA	1:B:445:LEU:HB2	1.95	0.47
1:B:252:MET:HG2	1:B:252:MET:H	1.40	0.47
1:A:110:ALA:HB1	1:A:229:VAL:HG12	1.97	0.47
1:B:80:THR:HG23	1:B:84:LEU:HD23	1.96	0.47
1:B:47:THR:HG23	1:B:51:ILE:HD13	1.96	0.46
1:A:258:VAL:HG21	1:A:336:VAL:HG21	1.97	0.46
1:A:354:THR:HG22	1:A:510:GLY:O	2.15	0.46
1:B:252:MET:HA	1:B:255:VAL:HB	1.97	0.46
1:B:93:ASP:HB3	1:B:249:GLY:HA2	1.97	0.46
1:B:351:LEU:HD13	1:B:555:ASN:HD22	1.81	0.46
1:B:463:TYR:HA	1:B:466:ILE:HD12	1.97	0.46
1:A:547:LEU:O	1:A:551:LEU:HB2	2.16	0.46
1:B:22:PRO:HD2	1:B:243:ARG:NH2	2.31	0.46
1:B:423:ILE:HA	1:B:479:ILE:HG13	1.98	0.45
1:B:207:VAL:O	1:B:211:VAL:HG23	2.16	0.45
1:A:359:LEU:HD11	1:A:388:TYR:HB2	1.98	0.45
1:B:347:ALA:HA	1:B:350:ILE:HD12	1.98	0.45
1:B:440:VAL:HG12	1:B:444:ARG:NE	2.31	0.45
1:B:63:MET:HE1	1:B:145:GLN:HB3	1.99	0.45
1:A:99:TYR:CD1	1:A:244:PHE:HE2	2.34	0.45
1:A:440:VAL:C	1:A:444:ARG:HE	2.25	0.45
1:A:419:PRO:HB3	1:A:489:ARG:HH12	1.82	0.44
1:A:32:ALA:HB3	1:A:241:ARG:CB	2.47	0.44
1:B:116:LEU:O	1:B:120:THR:HG23	2.17	0.44
1:B:552:VAL:HA	1:B:555:ASN:HB3	2.00	0.44
1:B:41:GLU:OE1	1:B:41:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ALA:HB1	1:B:361:THR:HB	1.99	0.44
1:B:461:GLY:HA2	1:B:464:LEU:HD12	1.99	0.44
1:A:413:TYR:HB2	1:A:414:PRO:HD3	1.99	0.43
1:A:176:ASP:HB3	1:A:179:GLU:HA	1.99	0.43
1:B:194:PHE:C	1:B:196:CYS:H	2.26	0.43
1:A:211:VAL:HA	1:A:215:VAL:HB	1.99	0.43
1:A:372:ARG:HH21	1:A:379:ILE:HG23	1.83	0.43
1:A:427:LEU:HB3	1:A:556:PHE:HB2	2.00	0.43
1:B:250:SER:HA	1:B:253:THR:OG1	2.18	0.43
1:A:349:CYS:HB2	1:A:506:THR:HG21	2.01	0.43
1:A:353:TRP:HB2	1:A:510:GLY:HA3	2.00	0.43
1:A:32:ALA:HA	1:A:35:ALA:HB3	2.00	0.43
1:B:146:LEU:HD22	1:B:150:TYR:HE1	1.83	0.43
1:A:389:VAL:HA	1:A:392:LEU:HD12	2.01	0.43
1:B:428:PHE:HE1	1:B:432:MET:HE3	1.83	0.43
1:B:382:ALA:C	1:B:384:MET:H	2.27	0.42
1:A:388:TYR:CZ	1:A:392:LEU:HD11	2.54	0.42
1:A:438:ALA:HB2	1:A:545:TYR:HB3	2.02	0.42
1:A:348:THR:HA	1:A:555:ASN:HD21	1.85	0.42
1:B:258:VAL:HG11	1:B:336:VAL:HG11	2.00	0.42
1:B:372:ARG:HH21	1:B:379:ILE:HG23	1.83	0.42
1:B:418:ARG:CB	1:B:422:ARG:HD3	2.49	0.42
1:B:440:VAL:O	1:B:444:ARG:HG3	2.19	0.42
1:A:109:GLN:HB3	1:A:159:GLY:HA3	2.01	0.42
1:A:466:ILE:N	1:A:467:PRO:HD2	2.35	0.42
1:A:80:THR:O	1:A:84:LEU:HD23	2.20	0.41
1:A:30:GLY:O	1:A:33:SER:HB3	2.20	0.41
1:A:215:VAL:HG12	1:A:219:TRP:CD1	2.55	0.41
1:B:263:TRP:HD1	1:B:264:ARG:NH2	2.18	0.41
1:A:37:ILE:HG22	1:A:167:VAL:HG13	2.02	0.41
1:A:93:ASP:HB3	1:A:249:GLY:CA	2.48	0.41
1:A:243:ARG:HD2	1:A:244:PHE:H	1.86	0.41
1:A:252:MET:H	1:A:252:MET:HG2	1.56	0.41
1:B:172:SER:HA	1:B:186:MET:HE1	2.02	0.41
1:B:121:ILE:HG13	1:B:122:ILE:HD12	2.02	0.41
1:A:95:PHE:CZ	1:A:96:LEU:HD12	2.55	0.41
1:A:418:ARG:N	1:A:419:PRO:HD3	2.36	0.41
1:B:28:THR:HG22	1:B:241:ARG:HA	2.01	0.41
1:B:239:THR:O	1:B:240:ASN:CB	2.69	0.41
1:A:58:TYR:HD1	1:A:217:ARG:HD3	1.86	0.40
1:A:93:ASP:OD1	1:A:98:ARG:NH2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:THR:O	1:A:358:GLN:HG2	2.21	0.40
1:B:354:THR:O	1:B:358:GLN:HG2	2.22	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%)	391 (85%)	48 (10%)	23 (5%)	1	17
1	B	462/590 (78%)	388 (84%)	60 (13%)	14 (3%)	3	26
All	All	924/1180 (78%)	779 (84%)	108 (12%)	37 (4%)	2	21

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	252	MET
1	A	411	PHE
1	A	413	TYR
1	A	419	PRO
1	A	493	LYS
1	B	96	LEU
1	B	240	ASN
1	B	371	ASP
1	A	22	PRO
1	A	177	GLU
1	A	371	ASP
1	A	372	ARG
1	A	383	SER
1	B	177	GLU
1	B	252	MET

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Mol	Chain	Res	Type
1	A	54	ASN
1	A	250	SER
1	A	401	ARG
1	A	499	SER
1	B	22	PRO
1	B	143	GLY
1	B	174	GLN
1	A	183	ARG
1	A	416	GLY
1	B	261	ALA
1	B	368	GLU
1	A	121	ILE
1	A	241	ARG
1	B	485	ASP
1	A	179	GLU
1	B	179	GLU
1	B	418	ARG
1	A	418	ARG
1	B	414	PRO
1	A	402	VAL
1	A	29	GLY

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%)	311 (81%)	75 (19%)	1	9
1	B	386/489 (79%)	301 (78%)	85 (22%)	1	7
All	All	772/978 (79%)	612 (79%)	160 (21%)	1	8

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	28	THR

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Mol	Chain	Res	Type
1	A	45	ARG
1	A	46	LEU
1	A	48	THR
1	A	49	LEU
1	A	55	LEU
1	A	56	VAL
1	A	57	THR
1	A	62	THR
1	A	69	THR
1	A	86	LEU
1	A	87	LEU
1	A	94	THR
1	A	96	LEU
1	A	109	GLN
1	A	111	THR
1	A	116	LEU
1	A	121	ILE
1	A	122	ILE
1	A	144	ILE
1	A	149	LEU
1	A	151	LEU
1	A	158	LEU
1	A	163	VAL
1	A	166	SER
1	A	168	SER
1	A	179	GLU
1	A	182	GLU
1	A	186	MET
1	A	195	PHE
1	A	196	CYS
1	A	202	LEU
1	A	207	VAL
1	A	208	LEU
1	A	218	LYS
1	A	230	LEU
1	A	232	LEU
1	A	234	VAL
1	A	243	ARG
1	A	248	ILE
1	A	252	MET
1	A	258	VAL
1	A	326	THR

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Mol	Chain	Res	Type
1	A	328	SER
1	A	330	LEU
1	A	338	GLN
1	A	339	ILE
1	A	351	LEU
1	A	355	VAL
1	A	359	LEU
1	A	363	SER
1	A	370	LEU
1	A	379	ILE
1	A	393	LEU
1	A	394	LEU
1	A	404	ILE
1	A	420	LEU
1	A	432	MET
1	A	442	LEU
1	A	462	PHE
1	A	465	LEU
1	A	487	PHE
1	A	496	LYS
1	A	498	MET
1	A	503	LEU
1	A	504	LEU
1	A	506	THR
1	A	517	LEU
1	A	525	THR
1	A	532	ILE
1	A	551	LEU
1	A	557	LEU
1	A	558	ILE
1	A	570	GLU
1	B	41	GLU
1	B	45	ARG
1	B	46	LEU
1	B	47	THR
1	B	48	THR
1	B	49	LEU
1	B	51	ILE
1	B	55	LEU
1	B	57	THR
1	B	69	THR
1	B	84	LEU

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Mol	Chain	Res	Type
1	B	86	LEU
1	B	87	LEU
1	B	94	THR
1	B	96	LEU
1	B	98	ARG
1	B	100	LEU
1	B	116	LEU
1	B	121	ILE
1	B	122	ILE
1	B	144	ILE
1	B	149	LEU
1	B	151	LEU
1	B	155	LEU
1	B	158	LEU
1	B	163	VAL
1	B	168	SER
1	B	172	SER
1	B	176	ASP
1	B	179	GLU
1	B	182	GLU
1	B	186	MET
1	B	196	CYS
1	B	205	VAL
1	B	208	LEU
1	B	223	ILE
1	B	232	LEU
1	B	247	LEU
1	B	252	MET
1	B	253	THR
1	B	254	GLN
1	B	258	VAL
1	B	259	ILE
1	B	260	VAL
1	B	264	ARG
1	B	266	ARG
1	B	269	GLU
1	B	326	THR
1	B	331	THR
1	B	335	GLU
1	B	339	ILE
1	B	345	ILE
1	B	348	THR

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Mol	Chain	Res	Type
1	B	354	THR
1	B	355	VAL
1	B	360	THR
1	B	362	LEU
1	B	369	THR
1	B	379	ILE
1	B	392	LEU
1	B	393	LEU
1	B	396	THR
1	B	420	LEU
1	B	422	ARG
1	B	425	LEU
1	B	442	LEU
1	B	445	LEU
1	B	447	THR
1	B	470	LEU
1	B	488	LEU
1	B	489	ARG
1	B	491	CYS
1	B	496	LYS
1	B	498	MET
1	B	503	LEU
1	B	506	THR
1	B	509	LEU
1	B	522	GLU
1	B	523	LYS
1	B	532	ILE
1	B	534	ASP
1	B	541	LEU
1	B	551	LEU
1	B	560	LEU
1	B	572	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	76	ASN
1	A	174	GLN
1	A	240	ASN
1	A	338	GLN
1	A	356	HIS

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Mol	Chain	Res	Type
1	A	483	GLN
1	A	537	ASN
1	A	555	ASN
1	B	67	ASN
1	B	254	GLN
1	B	483	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](#)

There are no ligands in this entry.

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%)	0.61	66 (14%) 6 8	3, 66, 230, 270	0
1	B	470/590 (79%)	0.66	60 (12%) 7 9	3, 57, 204, 239	0
All	All	940/1180 (79%)	0.63	126 (13%) 7 8	3, 60, 214, 270	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	ARG	7.8
1	B	486	PHE	5.8
1	A	329	THR	5.7
1	B	450	ALA	5.2
1	A	96	LEU	5.2
1	B	96	LEU	5.1
1	A	330	LEU	4.8
1	B	256	ALA	4.6
1	B	444	ARG	4.6
1	A	21	ARG	4.5
1	A	476	GLU	4.5
1	B	180	PRO	4.4
1	B	67	ASN	4.3
1	B	334	GLU	4.2
1	B	29	GLY	4.0
1	A	480	TYR	3.9
1	A	444	ARG	3.9
1	A	570	GLU	3.8
1	B	259	ILE	3.6
1	A	408	LYS	3.6
1	B	268	LEU	3.6
1	B	484	LEU	3.6
1	B	420	LEU	3.5
1	A	334	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	443	LYS	3.5
1	B	269	GLU	3.4
1	A	360	THR	3.4
1	B	342	MET	3.4
1	B	566	TYR	3.4
1	A	64	HIS	3.4
1	A	244	PHE	3.4
1	B	449	HIS	3.3
1	A	27	LYS	3.2
1	A	374	ILE	3.2
1	A	411	PHE	3.2
1	A	573	LEU	3.2
1	A	358	GLN	3.1
1	B	491	CYS	3.1
1	A	449	HIS	3.1
1	A	430	GLY	3.0
1	B	531	TRP	3.0
1	B	419	PRO	2.9
1	B	513	PHE	2.9
1	A	258	VAL	2.9
1	B	337	LYS	2.9
1	A	536	LEU	2.9
1	A	566	TYR	2.9
1	A	45	ARG	2.9
1	B	422	ARG	2.9
1	A	267	LYS	2.9
1	B	168	SER	2.8
1	B	358	GLN	2.8
1	B	41	GLU	2.8
1	A	489	ARG	2.7
1	A	540	ARG	2.7
1	B	368	GLU	2.7
1	B	369	THR	2.7
1	A	246	LYS	2.7
1	B	385	ALA	2.7
1	B	331	THR	2.7
1	B	497	GLY	2.7
1	A	567	VAL	2.6
1	A	259	ILE	2.6
1	A	564	LYS	2.6
1	B	383	SER	2.6
1	A	256	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	464	LEU	2.5
1	A	356	HIS	2.5
1	A	546	TRP	2.5
1	B	570	GLU	2.5
1	B	571	LYS	2.5
1	B	45	ARG	2.5
1	B	371	ASP	2.5
1	B	411	PHE	2.4
1	B	265	ASN	2.4
1	B	533	ALA	2.4
1	A	188	TYR	2.4
1	A	326	THR	2.4
1	A	447	THR	2.4
1	A	24	ASP	2.4
1	A	537	ASN	2.3
1	A	507	LEU	2.3
1	A	342	MET	2.3
1	B	490	GLU	2.3
1	B	386	VAL	2.3
1	A	249	GLY	2.3
1	A	542	TYR	2.3
1	A	30	GLY	2.3
1	A	369	THR	2.3
1	A	493	LYS	2.3
1	A	569	LYS	2.3
1	A	67	ASN	2.3
1	A	451	HIS	2.3
1	A	529	HIS	2.3
1	A	486	PHE	2.2
1	B	550	VAL	2.2
1	B	537	ASN	2.2
1	A	77	PHE	2.2
1	B	354	THR	2.2
1	A	195	PHE	2.2
1	A	511	PHE	2.2
1	A	450	ALA	2.2
1	B	68	ALA	2.2
1	B	441	GLU	2.2
1	A	446	ARG	2.2
1	B	563	SER	2.2
1	A	255	VAL	2.2
1	A	571	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	267	LYS	2.2
1	B	231	ALA	2.1
1	A	98	ARG	2.1
1	B	31	TRP	2.1
1	B	264	ARG	2.1
1	B	246	LYS	2.1
1	A	184	SER	2.1
1	B	572	ARG	2.1
1	A	550	VAL	2.1
1	B	260	VAL	2.1
1	B	573	LEU	2.1
1	B	382	ALA	2.1
1	B	77	PHE	2.1
1	A	572	ARG	2.1
1	A	412	ASN	2.1
1	B	423	ILE	2.0
1	A	409	LYS	2.0
1	B	24	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.