



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:25 PM GMT

PDB ID : 5A2N  
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](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.

---

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

MolProbity : 4.02b-467  
Mogul : unknown  
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

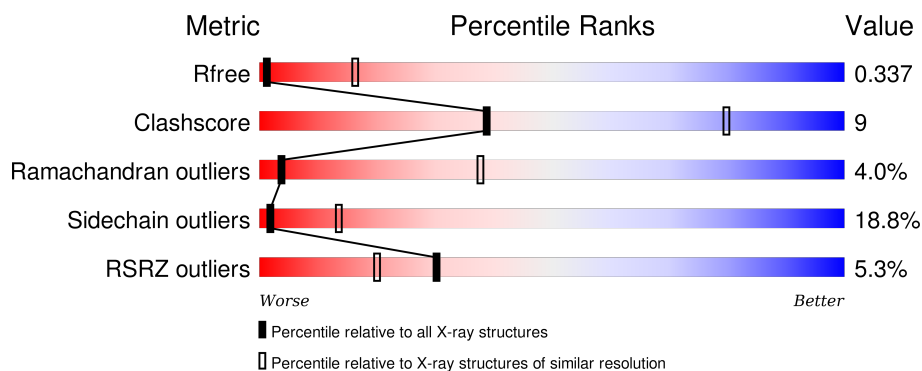
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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))
$R_{free}$	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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>4%</div> <div>52%</div> <div>23%</div> <div>• •</div> <div>20%</div> </div>
1	B	590	<div> <div>5%</div> <div>53%</div> <div>21%</div> <div>5%</div> <div>20%</div> </div>

## 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.

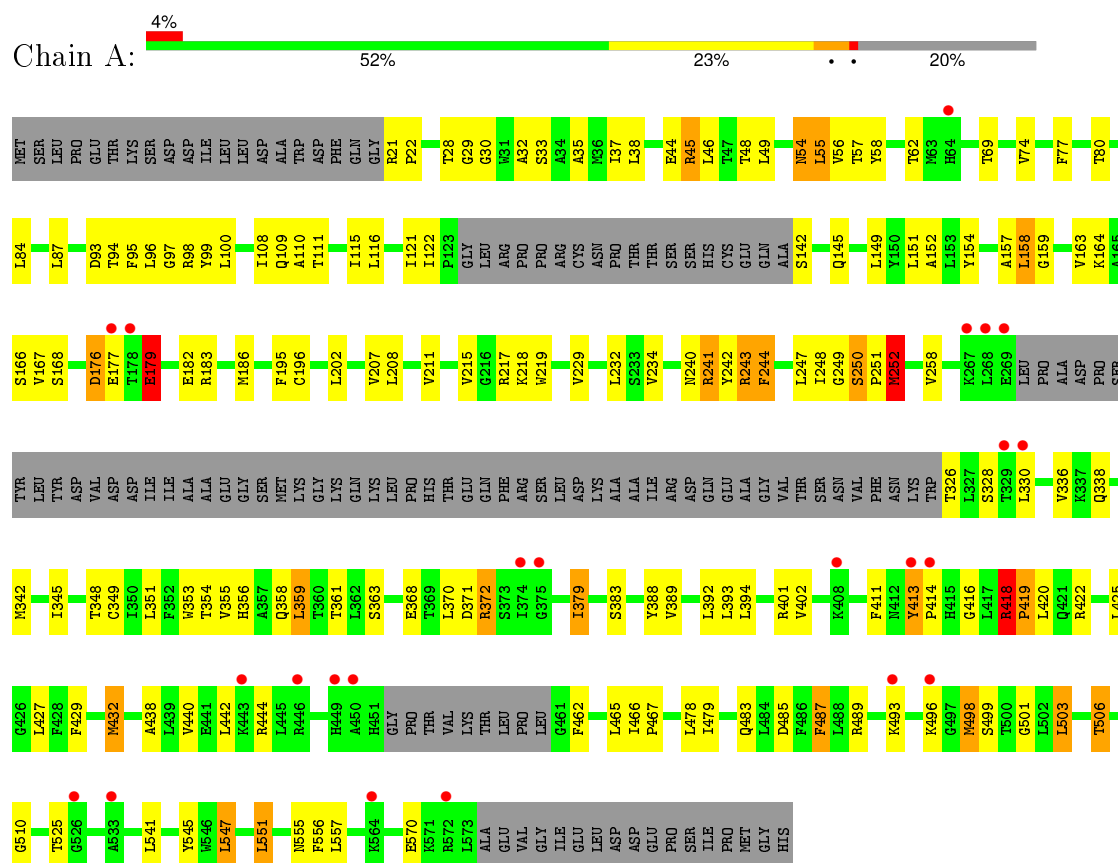
- Molecule 1 is a protein called PROTEIN NRT1/ PTR FAMILY 6.3.

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			

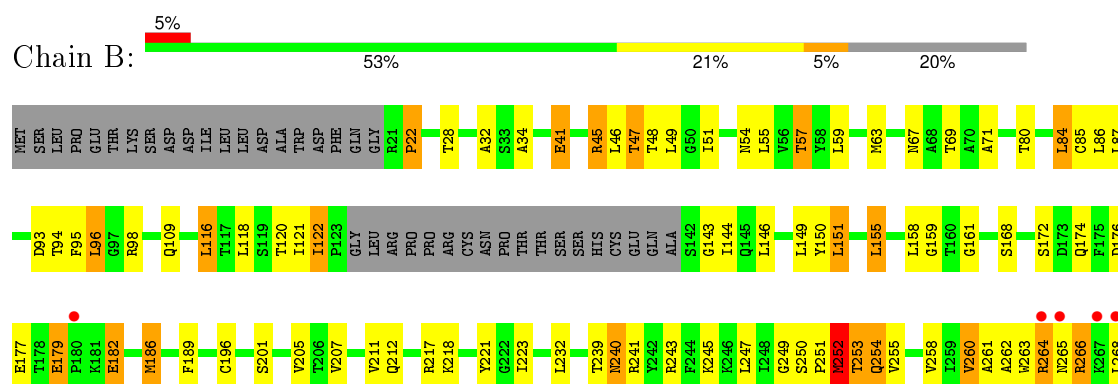
### 3 Residue-property plots

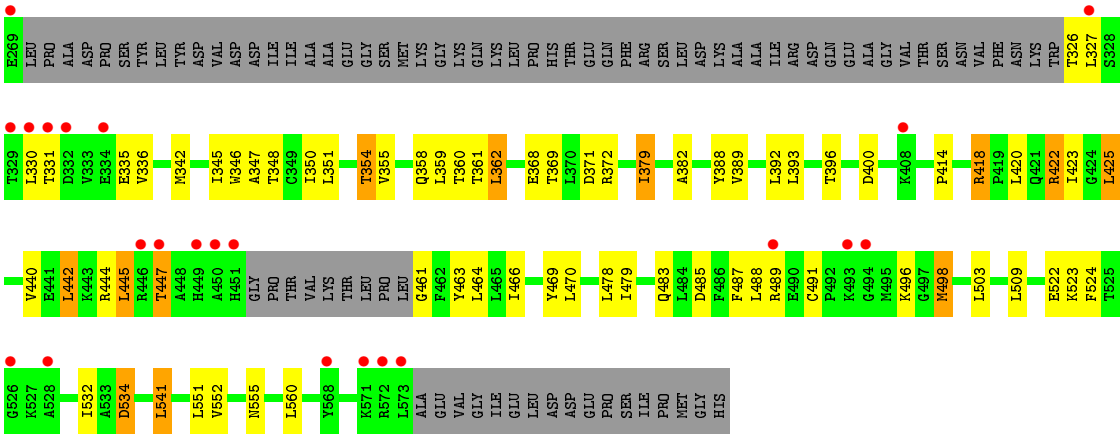
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PROTEIN NRT1/ PTR FAMILY 6.3



#### • 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, $\alpha$ , $\beta$ , $\gamma$	121.80Å 124.03Å 153.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.53 – 3.70 27.49 – 3.70	Depositor EDS
% Data completeness (in resolution range)	86.3 (27.53-3.70) 86.3 (27.49-3.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 3.74Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.278 , 0.310 0.299 , 0.337	Depositor DCC
$R_{free}$ test set	1103 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	105.4	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 109.6	EDS
Estimated twinning fraction	0.037 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	1 of 21857 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	7474	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.49	0/3734	0.77	1/5067 (0.0%)
1	B	0.52	0/3734	0.79	1/5067 (0.0%)
All	All	0.51	0/7468	0.78	2/10134 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	PHE	C-N-CA	5.29	134.92	121.70
1	A	97	GLY	C-N-CA	5.10	134.44	121.70

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	83	3786	66	0
1	B	3654	83	3786	68	0
All	All	7308	166	7572	134	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 9.

All (134) 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
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: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:A:240:ASN:C	1:A:242:TYR:H	2.11	0.53
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

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:205:VAL:HG21	1:B:389:VAL:HG21	1.92	0.51
1:A:345:ILE:O	1:A:348:THR:HG22	2.09	0.51
1:A:247:LEU:HG	1:A:248:ILE:N	2.26	0.51
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: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:B:212:GLN:HG2	1:B:217:ARG:HG3	1.95	0.48
1:A:250:SER:HB2	1:A:251:PRO:CA	2.42	0.48
1:A:32:ALA:CB	1:A:241:ARG:HB2	2.43	0.48
1:B:59:LEU:HA	1:B:63:MET:HB3	1.94	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:H	1:B:252:MET:HG2	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:B:252:MET:HA	1:B:255:VAL:HB	1.97	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: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:445:LEU:C	1:B:447:THR:H	2.19	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:501:GLY:C	1:A:503:LEU:H	2.20	0.45
1:A:99:TYR:CD1	1:A:244:PHE:HE2	2.34	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:461:GLY:HA2	1:B:464:LEU:HD12	1.99	0.44
1:B:71:ALA:HB1	1:B:361:THR:HB	1.99	0.44
1:B:41:GLU:OE1	1:B:41:GLU:HA	2.17	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: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:B:260:VAL:C	1:B:262:ALA:H	2.22	0.43
1:B:250:SER:HA	1:B:253:THR:OG1	2.18	0.43
1:A:427:LEU:HB3	1:A:556:PHE:HB2	2.00	0.43
1:A:353:TRP:HB2	1:A:510:GLY:HA3	2.00	0.43
1:A:349:CYS:HB2	1:A:506:THR:HG21	2.01	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:A:438:ALA:HB2	1:A:545:TYR:HB3	2.02	0.42
1:A:388:TYR:CZ	1:A:392:LEU:HD11	2.54	0.42
1:B:440:VAL:O	1:B:444:ARG:HG3	2.19	0.42
1:A:348:THR:HA	1:A:555:ASN:HD21	1.85	0.42
1:B:418:ARG:CB	1:B:422:ARG:HD3	2.49	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:A:466:ILE:N	1:A:467:PRO:HD2	2.35	0.42
1:A:109:GLN:HB3	1:A:159:GLY:HA3	2.01	0.42
1:A:80:THR:O	1:A:84:LEU:HD23	2.20	0.41
1:B:263:TRP:HD1	1:B:264:ARG:NH2	2.18	0.41
1:A:215:VAL:HG12	1:A:219:TRP:CD1	2.55	0.41
1:A:30:GLY:O	1:A:33:SER:HB3	2.20	0.41
1:A:93:ASP:HB3	1:A:249:GLY:CA	2.48	0.41
1:A:37:ILE:HG22	1:A:167:VAL:HG13	2.02	0.41
1:A:243:ARG:HD2	1:A:244:PHE:H	1.86	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:MET:HG2	1:A:252:MET:H	1.56	0.41
1:B:121:ILE:HG13	1:B:122:ILE:HD12	2.02	0.41
1:B:28:THR:HG22	1:B:241:ARG:HA	2.01	0.41
1:A:418:ARG:N	1:A:419:PRO:HD3	2.36	0.41
1:A:95:PHE:CZ	1:A:96:LEU:HD12	2.55	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
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

### 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%)	391 (85%)	48 (10%)	23 (5%)	3	31
1	B	462/590 (78%)	388 (84%)	60 (13%)	14 (3%)	5	46
All	All	924/1180 (78%)	779 (84%)	108 (12%)	37 (4%)	4	38

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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%)	318 (82%)	68 (18%)	2	16
1	B	386/489 (79%)	309 (80%)	77 (20%)	1	11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	772/978 (79%)	627 (81%)	145 (19%)	2 13

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	28	THR
1	A	38	LEU
1	A	45	ARG
1	A	46	LEU
1	A	48	THR
1	A	49	LEU
1	A	55	LEU
1	A	57	THR
1	A	62	THR
1	A	69	THR
1	A	87	LEU
1	A	94	THR
1	A	111	THR
1	A	116	LEU
1	A	122	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	176	ASP
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	232	LEU
1	A	234	VAL
1	A	243	ARG
1	A	244	PHE
1	A	252	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	326	THR
1	A	328	SER
1	A	330	LEU
1	A	338	GLN
1	A	351	LEU
1	A	355	VAL
1	A	359	LEU
1	A	363	SER
1	A	368	GLU
1	A	370	LEU
1	A	379	ILE
1	A	393	LEU
1	A	394	LEU
1	A	418	ARG
1	A	420	LEU
1	A	432	MET
1	A	442	LEU
1	A	462	PHE
1	A	465	LEU
1	A	485	ASP
1	A	487	PHE
1	A	496	LYS
1	A	498	MET
1	A	503	LEU
1	A	506	THR
1	A	525	THR
1	A	541	LEU
1	A	547	LEU
1	A	551	LEU
1	A	557	LEU
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	55	LEU
1	B	57	THR
1	B	69	THR
1	B	84	LEU
1	B	86	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	87	LEU
1	B	94	THR
1	B	96	LEU
1	B	98	ARG
1	B	116	LEU
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	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	218	LYS
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	260	VAL
1	B	264	ARG
1	B	266	ARG
1	B	326	THR
1	B	331	THR
1	B	335	GLU
1	B	345	ILE
1	B	348	THR
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	388	TYR
1	B	392	LEU
1	B	393	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	396	THR
1	B	400	ASP
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	487	PHE
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	509	LEU
1	B	522	GLU
1	B	523	LYS
1	B	524	PHE
1	B	532	ILE
1	B	534	ASP
1	B	541	LEU
1	B	551	LEU
1	B	560	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	483	GLN
1	A	555	ASN
1	B	54	ASN
1	B	67	ASN
1	B	72	ASN
1	B	212	GLN
1	B	254	GLN
1	B	483	GLN
1	B	543	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates 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, 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%)	-0.21	23 (4%)	33 22	3, 66, 230, 270	0
1	B	470/590 (79%)	-0.06	27 (5%)	27 17	3, 57, 204, 239	0
All	All	940/1180 (79%)	-0.13	50 (5%)	30 20	3, 60, 214, 270	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	LEU	5.7
1	A	329	THR	5.5
1	B	572	ARG	5.4
1	A	449	HIS	4.2
1	B	450	ALA	4.2
1	B	571	LYS	4.0
1	B	568	TYR	3.9
1	B	449	HIS	3.7
1	A	414	PRO	3.7
1	A	269	GLU	3.4
1	A	450	ALA	3.4
1	A	177	GLU	3.3
1	B	489	ARG	3.2
1	B	334	GLU	3.2
1	B	331	THR	3.1
1	A	267	LYS	3.1
1	B	330	LEU	3.0
1	B	180	PRO	3.0
1	B	451	HIS	2.9
1	A	413	TYR	2.9
1	A	446	ARG	2.9
1	B	573	LEU	2.7
1	A	493	LYS	2.7
1	B	268	LEU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	528	ALA	2.5
1	A	496	LYS	2.5
1	A	374	ILE	2.4
1	B	494	GLY	2.4
1	A	268	LEU	2.4
1	B	267	LYS	2.4
1	B	493	LYS	2.4
1	B	265	ASN	2.3
1	A	375	GLY	2.3
1	B	526	GLY	2.3
1	A	408	LYS	2.3
1	B	447	THR	2.3
1	B	327	LEU	2.3
1	A	533	ALA	2.2
1	B	264	ARG	2.2
1	A	178	THR	2.2
1	A	564	LYS	2.2
1	B	329	THR	2.2
1	A	572	ARG	2.2
1	A	64	HIS	2.1
1	A	443	LYS	2.1
1	B	269	GLU	2.1
1	B	446	ARG	2.1
1	B	332	ASP	2.1
1	B	408	LYS	2.1
1	A	526	GLY	2.1

## 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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.