Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 01:22 PM EST

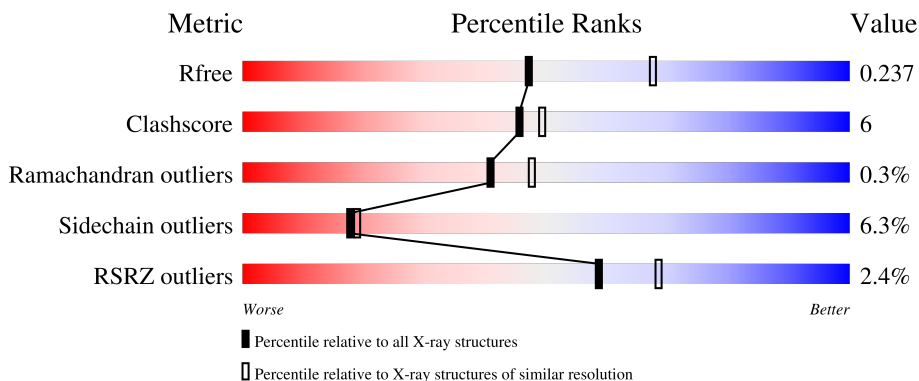|		
PDB ID	:	4Q7L
Title	:	Structure of NBD288 of TM287/288
Authors	:	Bukowska, M.A.; Hohl, M.; Gruetter, M.G.; Seeger, M.A.
Deposited on	:	2014-04-25
Resolution	:	2.35 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
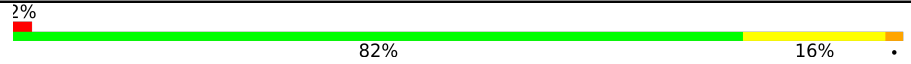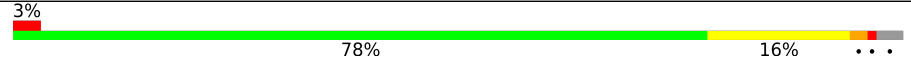*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	Percentile Ranks	Value
Rfree		0.237
Clashscore		6
Ramachandran outliers		0.3%
Sidechain outliers		6.3%
RSRZ outliers		2.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	256	2% 82% 16% ·
1	B	256	3% 78% 16% · · ·
1	C	256	2% 73% 19% · 7%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6168 atoms, of which 0 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 Uncharacterized ABC transporter ATP-binding protein TM_0288.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	2	0
			2039	1302	345	388	4			
1	B	248	Total	C	N	O	S	0	0	0
			1976	1267	333	372	4			
1	C	239	Total	C	N	O	S	0	3	0
			1934	1239	327	364	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	351	MET	-	initiating methionine	UNP Q9WYC4
A	352	SER	-	expression tag	UNP Q9WYC4
A	599	ALA	-	expression tag	UNP Q9WYC4
A	600	ALA	-	expression tag	UNP Q9WYC4
A	601	LEU	-	expression tag	UNP Q9WYC4
A	602	GLU	-	expression tag	UNP Q9WYC4
A	603	VAL	-	expression tag	UNP Q9WYC4
A	604	LEU	-	expression tag	UNP Q9WYC4
A	605	PHE	-	expression tag	UNP Q9WYC4
A	606	GLN	-	expression tag	UNP Q9WYC4
B	351	MET	-	initiating methionine	UNP Q9WYC4
B	352	SER	-	expression tag	UNP Q9WYC4
B	599	ALA	-	expression tag	UNP Q9WYC4
B	600	ALA	-	expression tag	UNP Q9WYC4
B	601	LEU	-	expression tag	UNP Q9WYC4
B	602	GLU	-	expression tag	UNP Q9WYC4
B	603	VAL	-	expression tag	UNP Q9WYC4
B	604	LEU	-	expression tag	UNP Q9WYC4
B	605	PHE	-	expression tag	UNP Q9WYC4
B	606	GLN	-	expression tag	UNP Q9WYC4
C	351	MET	-	initiating methionine	UNP Q9WYC4
C	352	SER	-	expression tag	UNP Q9WYC4
C	599	ALA	-	expression tag	UNP Q9WYC4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	600	ALA	-	expression tag	UNP Q9WYC4
C	601	LEU	-	expression tag	UNP Q9WYC4
C	602	GLU	-	expression tag	UNP Q9WYC4
C	603	VAL	-	expression tag	UNP Q9WYC4
C	604	LEU	-	expression tag	UNP Q9WYC4
C	605	PHE	-	expression tag	UNP Q9WYC4
C	606	GLN	-	expression tag	UNP Q9WYC4

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Ni 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total 111	O 111	0	0
3	B	47	Total 47	O 47	0	0
3	C	60	Total 60	O 60	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.

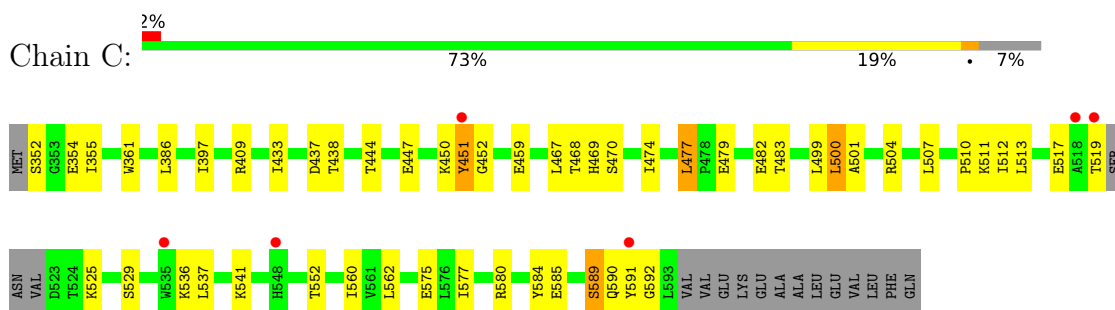• Molecule 1: Uncharacterized ABC transporter ATP-binding protein TM_0288
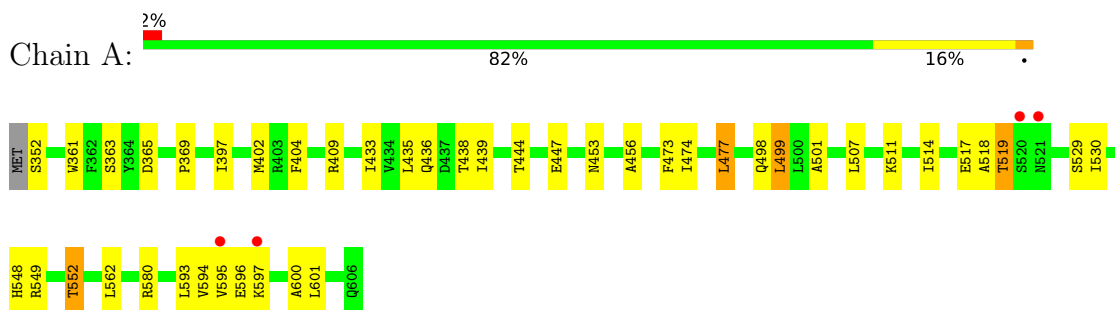
Chain A:

• Molecule 1: Uncharacterized ABC transporter ATP-binding protein TM_0288

Chain B:

• Molecule 1: Uncharacterized ABC transporter ATP-binding protein TM_0288

Chain C:
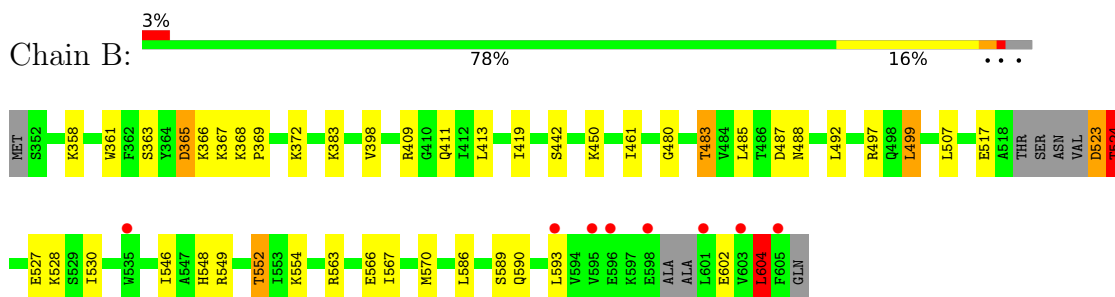
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	95.93Å 95.93Å 88.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.97 – 2.35 47.97 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.97-2.35) 99.3 (47.97-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1678)	Depositor
R, R_{free}	0.193 , 0.236 0.197 , 0.237	Depositor DCC
R_{free} test set	1885 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l 0.035 for h,-h-k,-l 0.015 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6168	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5411e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NI

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	0.29	0/2071	0.49	0/2792
1	B	0.26	0/2006	0.47	1/2699 (0.0%)
1	C	0.28	0/1967	0.44	0/2650
All	All	0.28	0/6044	0.47	1/8141 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	604	LEU	CA-CB-CG	5.14	127.12	115.30

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	2039	0	2090	23	0
1	B	1976	0	2035	26	1
1	C	1934	0	1976	28	0
2	B	1	0	0	0	0
3	A	111	0	0	4	0
3	B	47	0	0	4	1
3	C	60	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6168	0	6101	77	1

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 6.

All (77) 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:A:548:HIS:ND1	3:A:801:HOH:O	1.95	0.97
1:A:593:LEU:O	3:A:787:HOH:O	2.03	0.76
1:B:524:THR:OG1	3:B:847:HOH:O	2.06	0.73
1:B:383:LYS:NZ	3:B:837:HOH:O	2.23	0.71
1:A:580:ARG:HD2	3:A:792:HOH:O	1.90	0.70
1:B:411:GLN:OE1	3:B:831:HOH:O	2.09	0.69
1:B:567:ILE:HD13	1:B:570:MET:HE3	1.75	0.69
1:B:523:ASP:OD1	1:B:523:ASP:N	2.27	0.68
1:C:469:HIS:ND1	3:C:741:HOH:O	2.24	0.68
1:A:436:GLN:HG2	1:A:519:THR:HG23	1.77	0.67
1:B:365:ASP:HB3	1:B:367:LYS:HB2	1.79	0.65
1:A:595:VAL:HB	1:A:596:GLU:HG2	1.78	0.65
1:C:513:LEU:HD11	1:C:537:LEU:HG	1.80	0.64
1:C:354:GLU:OE2	3:C:743:HOH:O	2.15	0.63
1:C:438:THR:HG21	1:C:501:ALA:HB2	1.83	0.61
1:B:363:SER:O	1:B:366:LYS:NZ	2.33	0.61
1:C:467:LEU:HD22	1:C:536:LYS:HE2	1.82	0.60
1:A:438:THR:HG21	1:A:501:ALA:HB2	1.83	0.60
1:B:450:LYS:HG3	1:B:461:ILE:HD11	1.84	0.59
1:B:361:TRP:HB2	1:B:409:ARG:HB2	1.85	0.59
1:B:480:GLY:O	1:B:483:THR:OG1	2.20	0.59
1:A:363:SER:HB2	1:A:369:PRO:HA	1.89	0.55
1:B:590:GLN:HA	1:B:593:LEU:HD12	1.89	0.54
1:C:474:ILE:HA	1:C:477:LEU:HD22	1.89	0.54
1:B:398:VAL:HG21	1:B:546:ILE:HD11	1.90	0.53
1:A:433:ILE:HG22	1:A:514:ILE:HB	1.91	0.53
1:B:549:ARG:HB2	1:B:552:THR:HG23	1.91	0.52
1:B:487:ASP:N	1:B:488:ASN:HA	2.25	0.52
1:A:474:ILE:HA	1:A:477:LEU:HD22	1.92	0.51
1:B:363:SER:HB2	1:B:369:PRO:HA	1.93	0.51
1:C:451[A]:TYR:O	1:C:504:ARG:HG3	2.11	0.51
1:C:451[B]:TYR:O	1:C:504:ARG:HG3	2.11	0.50
1:C:468:THR:O	1:C:470:SER:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ILE:HD11	3:B:816:HOH:O	2.12	0.49
1:B:524:THR:HA	1:B:527:GLU:HB3	1.95	0.49
1:C:355:ILE:HD11	1:C:512:ILE:HD13	1.93	0.49
1:C:397:ILE:HD12	1:C:562:LEU:HD11	1.95	0.49
1:A:517:GLU:N	3:A:790:HOH:O	2.33	0.48
1:A:397:ILE:HD12	1:A:562:LEU:HD11	1.95	0.48
1:C:386:LEU:HD23	1:C:560:ILE:HB	1.96	0.48
1:C:447:GLU:HA	1:C:450:LYS:HB2	1.95	0.48
1:A:499:LEU:HD13	1:A:530:ILE:HG12	1.94	0.48
1:A:597:LYS:HE2	1:A:600:ALA:CB	2.45	0.47
1:A:361:TRP:HB2	1:A:409:ARG:HB2	1.97	0.46
1:A:402:MET:HE3	1:A:404:PHE:CE2	2.50	0.46
1:C:469:HIS:HB2	1:C:529:SER:HB3	1.97	0.46
1:B:442:SER:OG	1:B:488:ASN:HB3	2.15	0.46
1:B:524:THR:O	1:B:528:LYS:HG3	2.16	0.46
1:C:585:GLU:O	1:C:589:SER:OG	2.31	0.46
1:A:517:GLU:OE1	1:A:552:THR:HG21	2.16	0.45
1:C:590:GLN:O	1:C:592:GLY:N	2.45	0.45
1:B:368:LYS:HA	1:B:369:PRO:HD3	1.81	0.45
1:A:549:ARG:HB2	1:A:552:THR:HG23	1.97	0.45
1:B:548:HIS:HA	1:B:604:LEU:HD21	1.99	0.44
1:C:361:TRP:HB2	1:C:409:ARG:HB2	2.00	0.44
1:C:437:ASP:OD1	1:C:438:THR:N	2.50	0.44
1:B:492:LEU:O	1:B:497:ARG:NH1	2.51	0.43
1:C:451[A]:TYR:CD1	1:C:452:GLY:HA2	2.53	0.43
1:C:517:GLU:OE2	1:C:552:THR:HG21	2.18	0.43
1:B:499:LEU:HD13	1:B:530:ILE:HG12	2.00	0.42
1:C:580:ARG:HG3	1:C:584:TYR:CD1	2.53	0.42
1:A:597:LYS:HE2	1:A:600:ALA:HB2	2.01	0.42
1:A:498:GLN:HE22	1:A:518:ALA:HA	1.84	0.42
1:B:358:LYS:HB2	1:B:411:GLN:HG3	2.01	0.42
1:A:352:SER:HB2	1:A:511:LYS:HD2	2.01	0.41
1:C:352:SER:HB2	1:C:511:LYS:HD2	2.02	0.41
1:B:372:LYS:HG3	1:B:566:GLU:HG2	2.02	0.41
1:C:438:THR:HB	3:C:722:HOH:O	2.19	0.41
1:C:510:PRO:HD2	1:C:541:LYS:HE2	2.02	0.41
1:A:444:THR:OG1	1:A:447:GLU:HG2	2.20	0.40
1:A:595:VAL:HA	1:A:596:GLU:HA	1.83	0.40
1:B:499:LEU:HD12	1:B:499:LEU:HA	1.90	0.40
1:C:451[A]:TYR:HA	1:C:452:GLY:HA2	1.83	0.40
1:C:500:LEU:HD12	1:C:500:LEU:HA	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:LYS:HA	1:C:536:LYS:HD2	1.88	0.40
1:C:444:THR:HA	1:C:483:THR:O	2.21	0.40
1:A:453:ASN:ND2	1:A:456:ALA:HB2	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:SER:O	3:B:822:HOH:O[3_575]	1.97	0.23

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	255/256 (100%)	248 (97%)	7 (3%)	0	100	100
1	B	242/256 (94%)	235 (97%)	6 (2%)	1 (0%)	34	38
1	C	238/256 (93%)	228 (96%)	9 (4%)	1 (0%)	34	38
All	All	735/768 (96%)	711 (97%)	22 (3%)	2 (0%)	41	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	591	TYR
1	B	524	THR

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	225/224 (100%)	213 (95%)	12 (5%)	22	26
1	B	218/224 (97%)	203 (93%)	15 (7%)	15	15
1	C	212/224 (95%)	196 (92%)	16 (8%)	13	13
All	All	655/672 (98%)	612 (93%)	43 (7%)	18	17

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	ASP
1	A	435	LEU
1	A	439	ILE
1	A	473	PHE
1	A	477	LEU
1	A	499	LEU
1	A	507	LEU
1	A	519	THR
1	A	529	SER
1	A	552	THR
1	A	594	VAL
1	A	601	LEU
1	B	365	ASP
1	B	413	LEU
1	B	483	THR
1	B	485	LEU
1	B	499	LEU
1	B	507	LEU
1	B	517	GLU
1	B	523	ASP
1	B	524	THR
1	B	552	THR
1	B	554	LYS
1	B	563	ARG
1	B	586	LEU
1	B	602	GLU
1	B	604	LEU
1	C	433	ILE
1	C	451[A]	TYR
1	C	451[B]	TYR
1	C	459	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	477	LEU
1	C	479	GLU
1	C	482	GLU
1	C	499	LEU
1	C	500	LEU
1	C	507	LEU
1	C	519	THR
1	C	525	LYS
1	C	575[A]	GLU
1	C	575[B]	GLU
1	C	577	ILE
1	C	589	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	411	GLN
1	B	494	GLN
1	C	411	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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, 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	255/256 (99%)	-0.08	4 (1%)	72	80	25, 45, 87, 119	0
1	B	248/256 (96%)	0.01	8 (3%)	47	59	38, 58, 98, 117	0
1	C	239/256 (93%)	-0.01	6 (2%)	57	67	30, 53, 92, 109	0
All	All	742/768 (96%)	-0.03	18 (2%)	59	68	25, 53, 92, 119	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	595	VAL	5.2
1	C	519	THR	4.6
1	C	451[A]	TYR	4.0
1	A	521	ASN	3.9
1	A	520	SER	3.9
1	B	603	VAL	3.6
1	C	518	ALA	3.5
1	C	591	TYR	3.0
1	B	595	VAL	2.9
1	C	535[A]	TRP	2.8
1	B	596	GLU	2.5
1	B	535	TRP	2.4
1	B	593	LEU	2.3
1	B	598	GLU	2.3
1	B	601	LEU	2.2
1	A	597	LYS	2.1
1	B	605	PHE	2.1
1	C	548	HIS	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 (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(Å^2)	Q<0.9
2	NI	B	701	1/1	0.97	0.15	64,64,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.