



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:56 PM GMT

PDB ID : 3V89
Title : The crystal structure of transferrin binding protein A (TbpA) from *Neisseria meningitidis* serogroup B in complex with the C-lobe of human transferrin
Authors : Noinaj, N.; Oke, M.; Easley, N.; Zak, O.; Aisen, P.; Buchanan, S.K.
Deposited on : 2011-12-22
Resolution : 3.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

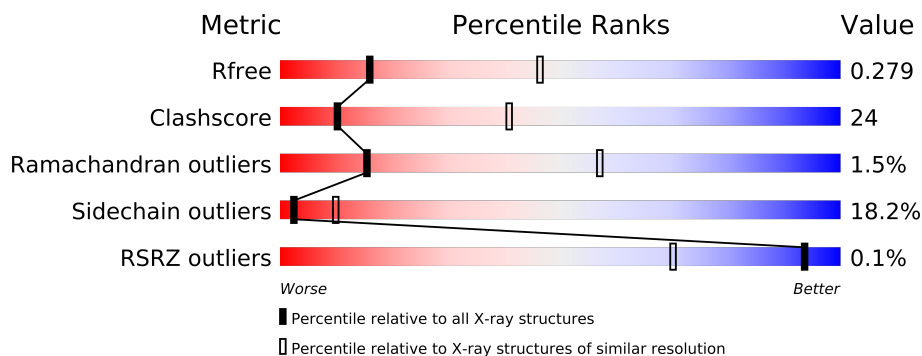
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.10 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}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	904	
2	B	343	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9110 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Transferrin-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	853	Total	C	N	O	S	0	0	0
			6558	4091	1182	1274	11			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	EXPRESSION TAG	UNP Q9JPJ0
A	13	ASP	-	EXPRESSION TAG	UNP Q9JPJ0
A	14	ILE	-	EXPRESSION TAG	UNP Q9JPJ0
A	15	HIS	-	EXPRESSION TAG	UNP Q9JPJ0
A	16	HIS	-	EXPRESSION TAG	UNP Q9JPJ0
A	17	HIS	-	EXPRESSION TAG	UNP Q9JPJ0
A	18	HIS	-	EXPRESSION TAG	UNP Q9JPJ0
A	19	HIS	-	EXPRESSION TAG	UNP Q9JPJ0
A	20	HIS	-	EXPRESSION TAG	UNP Q9JPJ0
A	21	HIS	-	EXPRESSION TAG	UNP Q9JPJ0
A	22	HIS	-	EXPRESSION TAG	UNP Q9JPJ0
A	23	HIS	-	EXPRESSION TAG	UNP Q9JPJ0
A	24	HIS	-	EXPRESSION TAG	UNP Q9JPJ0

- Molecule 2 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	339	Total	C	N	O	S	0	0	0
			2552	1587	436	503	26			

There is a discrepancy between the modelled and reference sequences:

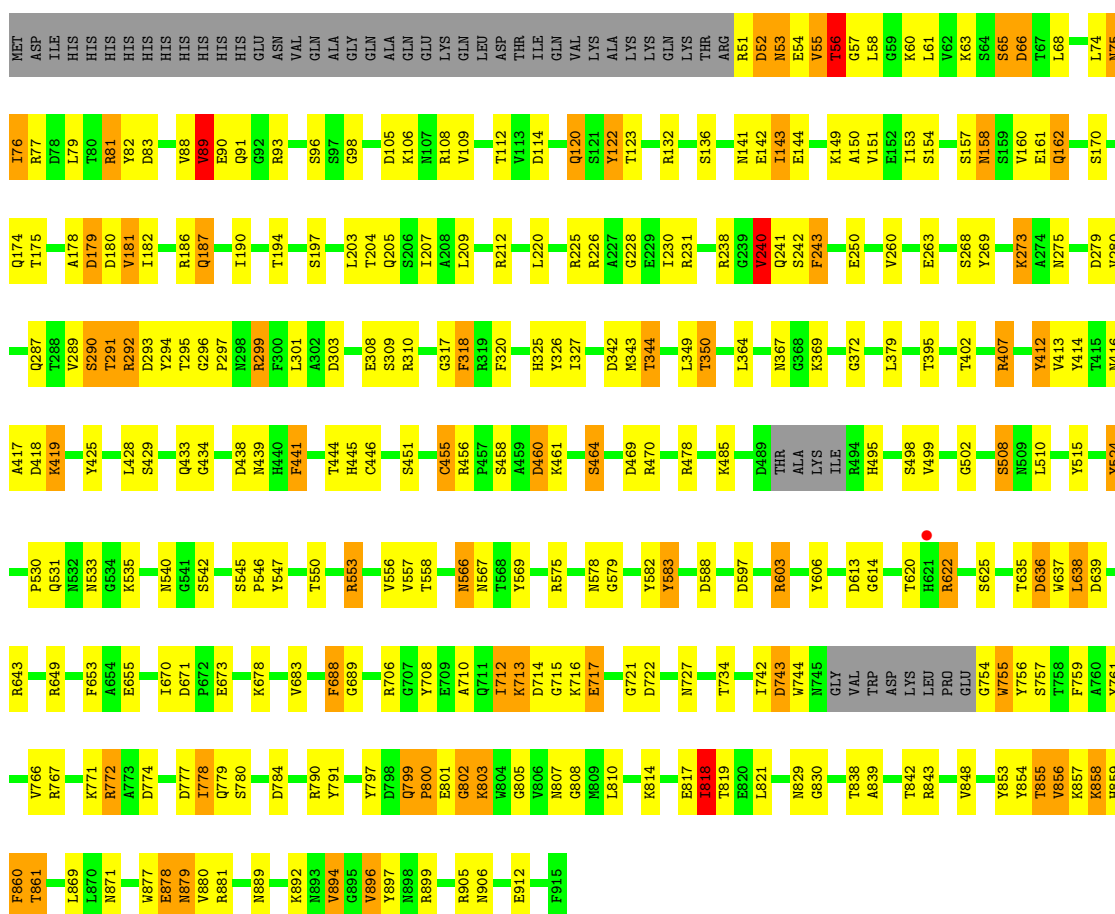
Chain	Residue	Modelled	Actual	Comment	Reference
B	429	VAL	ILE	VARIANT	UNP P02787

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.

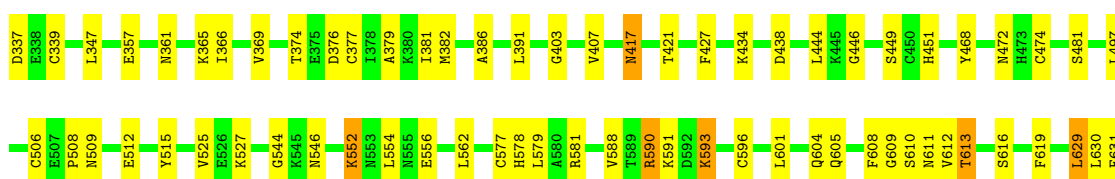
• Molecule 1: Transferrin-binding protein A

Chain A: 



• Molecule 2: Serotransferrin

Chain B: 



R632	
L641	
N645	
E648	
E653	
Y656	
K657	
T667	
C674	
T675	
PHE	
ARG	
ARG	
PRO	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.05Å 107.59Å 130.72Å 90.00° 94.48° 90.00°	Depositor
Resolution (Å)	29.96 – 3.10 41.69 – 3.09	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.96-3.10) 91.6 (41.69-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_865)	Depositor
R, R_{free}	0.224 , 0.287 0.221 , 0.279	Depositor DCC
R_{free} test set	1345 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 28386 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9110	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.31	0/6701	0.57	0/9081
2	B	0.28	0/2605	0.50	0/3535
All	All	0.30	0/9306	0.55	0/12616

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	VAL	Peptide
1	A	743	ASP	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6558	0	37	190	1
2	B	2552	0	0	28	1
All	All	9110	0	37	215	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (215) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:75:ASN:ND2	1:A:77:ARG:N	1.95	1.14
1:A:854:TYR:CE1	1:A:856:VAL:CG1	2.30	1.13
1:A:52:ASP:CB	1:A:53:ASN:CB	2.30	1.09
1:A:854:TYR:CD1	1:A:856:VAL:CG1	2.40	1.05
1:A:855:THR:CG2	1:A:861:THR:CB	2.37	1.03
1:A:75:ASN:C	1:A:75:ASN:HD22	1.61	1.02
1:A:75:ASN:ND2	1:A:76:ILE:N	2.09	1.01
1:A:717:GLU:OE2	1:A:829:ASN:N	1.94	1.00
1:A:75:ASN:HD22	1:A:76:ILE:N	1.63	0.95
1:A:854:TYR:HE1	1:A:856:VAL:CB	1.81	0.93
1:A:75:ASN:HD21	1:A:77:ARG:N	1.67	0.91
1:A:294:TYR:OH	1:A:297:PRO:O	1.88	0.91
1:A:291:THR:O	1:A:294:TYR:N	2.06	0.88
1:A:821:LEU:HD21	1:A:877:TRP:CH2	2.08	0.88
1:A:869:LEU:O	1:A:905:ARG:NH1	2.08	0.87
1:A:854:TYR:HE1	1:A:856:VAL:CA	1.89	0.85
2:B:497:LEU:O	2:B:527:LYS:NZ	2.09	0.85
1:A:854:TYR:HE1	1:A:856:VAL:CG1	1.84	0.85
1:A:456:ARG:O	1:A:461:LYS:NZ	2.10	0.84
1:A:75:ASN:ND2	1:A:75:ASN:C	2.30	0.84
1:A:854:TYR:CE1	1:A:856:VAL:CA	2.63	0.81
1:A:364:LEU:O	1:A:367:ASN:ND2	2.15	0.79
1:A:161:GLU:O	1:A:162:GLN:NE2	2.16	0.79
1:A:179:ASP:OD1	1:A:212:ARG:NH2	2.15	0.79
1:A:75:ASN:HD22	1:A:77:ARG:N	1.77	0.78
1:A:194:THR:OG1	1:A:205:GLN:OE1	2.02	0.78
1:A:779:GLN:OE1	1:A:780:SER:N	2.18	0.77
1:A:268:SER:OG	1:A:269:TYR:N	2.19	0.76
1:A:54:GLU:O	1:A:55:VAL:CB	2.34	0.75
1:A:754:GLY:O	1:A:797:TYR:CD1	2.39	0.75
1:A:114:ASP:OD2	1:A:175:THR:OG1	2.04	0.75
1:A:174:GLN:OE1	1:A:174:GLN:N	2.20	0.75
1:A:105:ASP:OD2	1:A:881:ARG:NH2	2.21	0.74
1:A:802:GLY:O	1:A:803:LYS:CB	2.36	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:805:GLY:CA	1:A:853:TYR:CE2	2.73	0.71
1:A:807:ASN:OD1	1:A:808:GLY:N	2.23	0.71
1:A:754:GLY:O	1:A:755:TRP:CB	2.39	0.69
1:A:613:ASP:OD1	1:A:614:GLY:N	2.26	0.69
1:A:318:PHE:N	1:A:318:PHE:CD2	2.60	0.69
1:A:269:TYR:OH	1:A:546:PRO:O	2.11	0.68
1:A:412:TYR:CD2	1:A:412:TYR:C	2.67	0.68
1:A:53:ASN:C	1:A:53:ASN:OD1	2.33	0.68
1:A:291:THR:O	1:A:293:ASP:N	2.26	0.68
1:A:553:ARG:NH2	1:A:553:ARG:CG	2.57	0.67
2:B:357:GLU:O	2:B:361:ASN:ND2	2.29	0.66
1:A:108:ARG:NH2	1:A:673:GLU:OE2	2.29	0.65
2:B:403:GLY:O	2:B:591:LYS:NZ	2.30	0.65
1:A:801:GLU:O	1:A:803:LYS:N	2.30	0.65
1:A:799:GLN:O	1:A:802:GLY:N	2.30	0.65
1:A:878:GLU:N	1:A:879:ASN:O	2.29	0.65
1:A:854:TYR:HD1	1:A:856:VAL:CG1	2.02	0.64
1:A:810:LEU:HD23	1:A:810:LEU:O	1.97	0.64
1:A:688:PHE:CD2	1:A:688:PHE:N	2.63	0.64
1:A:821:LEU:CD2	1:A:877:TRP:CH2	2.80	0.63
1:A:89:VAL:CG1	1:A:89:VAL:O	2.46	0.63
1:A:688:PHE:O	1:A:743:ASP:N	2.31	0.63
2:B:546:ASN:O	2:B:552:LYS:CG	2.47	0.63
2:B:544:GLY:O	2:B:552:LYS:NZ	2.32	0.62
1:A:461:LYS:O	1:A:464:SER:OG	2.16	0.62
2:B:590:ARG:NH1	2:B:590:ARG:CG	2.63	0.62
2:B:468:TYR:O	2:B:472:ASN:N	2.33	0.62
1:A:854:TYR:CE1	1:A:856:VAL:N	2.69	0.61
1:A:242:SER:O	1:A:287:GLN:O	2.17	0.61
1:A:160:VAL:O	1:A:603:ARG:NH2	2.32	0.61
1:A:342:ASP:OD2	1:A:344:THR:N	2.34	0.60
1:A:801:GLU:O	1:A:802:GLY:C	2.39	0.60
2:B:386:ALA:O	2:B:590:ARG:NH2	2.35	0.59
1:A:578:ASN:OD1	1:A:579:GLY:N	2.34	0.59
1:A:243:PHE:CD2	1:A:243:PHE:O	2.56	0.59
1:A:56:THR:OG1	1:A:57:GLY:N	2.31	0.59
2:B:446:GLY:O	2:B:481:SER:OG	2.20	0.59
1:A:228:GLY:O	1:A:231:ARG:NH1	2.36	0.59
1:A:712:ILE:O	1:A:713:LYS:NZ	2.36	0.58
1:A:77:ARG:NH2	1:A:90:GLU:OE2	2.36	0.58
1:A:799:GLN:O	1:A:800:PRO:C	2.42	0.58
1:A:187:GLN:OE1	1:A:212:ARG:O	2.21	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:854:TYR:CD1	1:A:856:VAL:N	2.73	0.57
1:A:533:ASN:N	1:A:533:ASN:OD1	2.37	0.57
1:A:860:PHE:CD2	1:A:860:PHE:N	2.73	0.57
1:A:829:ASN:CG	1:A:830:GLY:N	2.57	0.57
1:A:441:PHE:CD2	1:A:441:PHE:C	2.78	0.57
1:A:114:ASP:OD2	1:A:407:ARG:NH2	2.38	0.56
1:A:896:VAL:CG1	1:A:897:TYR:N	2.68	0.56
1:A:566:ASN:OD1	1:A:566:ASN:N	2.37	0.56
1:A:240:VAL:O	1:A:241:GLN:CG	2.53	0.56
1:A:778:ILE:N	1:A:778:ILE:CD1	2.69	0.56
1:A:530:PRO:CA	1:A:531:GLN:CB	2.84	0.56
1:A:162:GLN:CG	1:A:170:SER:OG	2.54	0.56
1:A:74:LEU:O	1:A:225:ARG:NH1	2.38	0.56
1:A:296:GLY:N	1:A:343:MET:O	2.39	0.56
1:A:243:PHE:CG	1:A:243:PHE:O	2.58	0.56
1:A:671:ASP:O	1:A:727:ASN:ND2	2.39	0.56
1:A:445:HIS:O	1:A:445:HIS:CD2	2.60	0.55
1:A:154:SER:OG	1:A:158:ASN:OD1	2.24	0.55
1:A:150:ALA:N	1:A:174:GLN:NE2	2.54	0.55
1:A:263:GLU:OE2	1:A:372:GLY:N	2.39	0.55
1:A:649:ARG:NH1	1:A:673:GLU:OE1	2.40	0.55
1:A:418:ASP:OD1	1:A:419:LYS:N	2.39	0.55
1:A:649:ARG:NH2	1:A:655:GLU:OE1	2.41	0.54
2:B:610:SER:O	2:B:613:THR:OG1	2.25	0.54
1:A:877:TRP:CD1	1:A:877:TRP:O	2.61	0.54
1:A:238:ARG:O	1:A:240:VAL:CG2	2.54	0.54
1:A:508:SER:CB	1:A:653:PHE:CD2	2.90	0.54
1:A:294:TYR:CG	1:A:295:THR:N	2.75	0.54
1:A:784:ASP:OD1	1:A:881:ARG:NH1	2.40	0.54
1:A:65:SER:N	1:A:149:LYS:O	2.41	0.54
1:A:635:THR:O	1:A:636:ASP:CB	2.56	0.53
1:A:52:ASP:OD1	1:A:53:ASN:CB	2.56	0.53
1:A:308:GLU:OE2	1:A:310:ARG:NH2	2.42	0.53
1:A:325:HIS:CD2	1:A:414:TYR:CD1	2.97	0.52
1:A:88:VAL:O	1:A:98:GLY:O	2.26	0.52
1:A:743:ASP:O	1:A:744:TRP:C	2.48	0.52
1:A:174:GLN:CD	1:A:174:GLN:N	2.62	0.52
2:B:449:SER:OG	2:B:451:HIS:NE2	2.42	0.52
1:A:81:ARG:CD	1:A:82:TYR:CE2	2.92	0.52
1:A:150:ALA:N	1:A:174:GLN:CG	2.72	0.52
1:A:96:SER:OG	1:A:142:GLU:OE2	2.28	0.52
1:A:857:LYS:O	1:A:859:HIS:N	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:294:TYR:CD1	1:A:295:THR:N	2.79	0.51
1:A:810:LEU:HD23	1:A:810:LEU:C	2.31	0.51
1:A:66:ASP:OD1	1:A:66:ASP:N	2.42	0.51
1:A:714:ASP:N	1:A:715:GLY:CA	2.74	0.51
1:A:144:GLU:OE1	1:A:225:ARG:NH2	2.43	0.51
1:A:613:ASP:CG	1:A:614:GLY:N	2.64	0.51
1:A:540:ASN:O	2:B:434:LYS:NZ	2.44	0.50
1:A:89:VAL:O	1:A:96:SER:O	2.29	0.50
1:A:502:GLY:CA	1:A:583:TYR:CE2	2.95	0.50
1:A:51:ARG:O	1:A:52:ASP:O	2.30	0.50
2:B:381:ILE:O	2:B:590:ARG:CZ	2.60	0.50
1:A:547:TYR:OH	2:B:434:LYS:NZ	2.45	0.50
1:A:53:ASN:O	1:A:53:ASN:OD1	2.30	0.49
1:A:143:ILE:CD1	1:A:143:ILE:N	2.75	0.49
1:A:638:LEU:CD2	1:A:639:ASP:N	2.76	0.49
1:A:688:PHE:CD2	1:A:689:GLY:N	2.80	0.49
1:A:178:ALA:O	1:A:181:VAL:CG2	2.61	0.49
1:A:756:TYR:CD1	1:A:757:SER:N	2.81	0.48
1:A:55:VAL:O	1:A:56:THR:O	2.30	0.48
1:A:93:ARG:NH1	1:A:889:ASN:ND2	2.62	0.48
1:A:734:THR:OG1	1:A:767:ARG:NE	2.46	0.48
1:A:279:ASP:OD1	1:A:369:LYS:NZ	2.47	0.48
1:A:52:ASP:CA	1:A:53:ASN:CB	2.91	0.47
1:A:52:ASP:CG	1:A:53:ASN:CB	2.83	0.47
1:A:800:PRO:O	1:A:801:GLU:CB	2.62	0.47
1:A:242:SER:O	1:A:243:PHE:CD1	2.67	0.47
1:A:122:TYR:O	1:A:136:SER:OG	2.32	0.47
2:B:629:LEU:C	2:B:631:PHE:N	2.67	0.47
1:A:317:GLY:C	1:A:318:PHE:CD2	2.87	0.47
1:A:469:ASP:OD1	1:A:569:TYR:OH	2.32	0.47
1:A:240:VAL:C	1:A:241:GLN:CG	2.83	0.47
1:A:799:GLN:O	1:A:801:GLU:N	2.47	0.47
1:A:542:SER:O	1:A:545:SER:N	2.48	0.47
1:A:433:GLN:CG	1:A:434:GLY:N	2.78	0.47
2:B:653:GLU:O	2:B:656:VAL:O	2.32	0.46
1:A:636:ASP:O	1:A:637:TRP:CB	2.63	0.46
1:A:877:TRP:O	1:A:878:GLU:CD	2.54	0.46
1:A:416:ASN:OD1	1:A:417:ALA:N	2.48	0.46
1:A:446:CYS:SG	1:A:455:CYS:C	2.94	0.46
1:A:60:LYS:CB	1:A:153:ILE:O	2.64	0.46
1:A:838:THR:CG2	1:A:839:ALA:N	2.78	0.46
1:A:821:LEU:HD21	1:A:877:TRP:CZ2	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:605:GLN:O	2:B:609:GLY:N	2.49	0.46
2:B:376:ASP:OD1	2:B:377:CYS:N	2.49	0.46
1:A:290:SER:O	1:A:291:THR:OG1	2.35	0.45
1:A:524:TYR:CD2	1:A:524:TYR:C	2.90	0.45
1:A:458:SER:OG	1:A:460:ASP:OD2	2.35	0.45
1:A:122:TYR:CD2	1:A:122:TYR:C	2.91	0.45
1:A:856:VAL:CG2	1:A:856:VAL:O	2.66	0.44
1:A:713:LYS:C	1:A:715:GLY:CA	2.85	0.44
2:B:590:ARG:NE	2:B:593:LYS:NZ	2.65	0.44
1:A:412:TYR:CD2	1:A:413:VAL:N	2.85	0.44
1:A:273:LYS:O	1:A:273:LYS:CD	2.64	0.44
1:A:291:THR:O	1:A:292:ARG:C	2.57	0.43
1:A:756:TYR:CD1	1:A:756:TYR:C	2.92	0.43
1:A:706:ARG:NH2	1:A:777:ASP:OD2	2.51	0.43
1:A:896:VAL:O	1:A:897:TYR:CB	2.66	0.43
1:A:653:PHE:N	1:A:653:PHE:CD1	2.86	0.43
1:A:622:ARG:N	1:A:622:ARG:CD	2.81	0.43
2:B:379:ALA:O	2:B:382:MET:N	2.52	0.43
1:A:294:TYR:CZ	1:A:297:PRO:O	2.71	0.42
1:A:120:GLN:NE2	1:A:653:PHE:CZ	2.87	0.42
1:A:416:ASN:C	1:A:416:ASN:OD1	2.57	0.42
1:A:759:PHE:C	1:A:759:PHE:CD2	2.92	0.42
1:A:761:TYR:CE1	1:A:791:TYR:CZ	3.07	0.42
1:A:721:GLY:O	2:B:365:LYS:NZ	2.53	0.42
2:B:427:PHE:CE2	2:B:578:HIS:CE1	3.08	0.42
1:A:502:GLY:N	1:A:583:TYR:CE2	2.87	0.42
1:A:75:ASN:ND2	1:A:76:ILE:CA	2.80	0.42
2:B:508:PRO:O	2:B:515:TYR:CE1	2.73	0.42
1:A:582:TYR:C	1:A:582:TYR:CD1	2.93	0.42
1:A:326:TYR:CD1	1:A:327:ILE:N	2.88	0.42
2:B:337:ASP:O	2:B:339:CYS:N	2.53	0.42
1:A:742:ILE:CD1	1:A:744:TRP:NE1	2.83	0.41
2:B:608:PHE:CD1	2:B:619:PHE:CD2	3.08	0.41
1:A:120:GLN:NE2	1:A:653:PHE:CE2	2.89	0.41
1:A:643:ARG:NH2	1:A:643:ARG:CG	2.82	0.41
1:A:606:TYR:C	1:A:606:TYR:CD2	2.92	0.41
1:A:857:LYS:O	1:A:858:LYS:C	2.58	0.41
1:A:710:ALA:N	1:A:774:ASP:O	2.53	0.41
1:A:187:GLN:CG	1:A:187:GLN:O	2.69	0.41
1:A:342:ASP:OD2	1:A:342:ASP:C	2.58	0.41
1:A:855:THR:O	1:A:856:VAL:C	2.59	0.41
1:A:425:TYR:O	1:A:485:LYS:N	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:649:ARG:NH1	1:A:673:GLU:CD	2.74	0.41
2:B:417:ASN:N	2:B:417:ASN:OD1	2.53	0.41
1:A:451:SER:OG	1:A:451:SER:O	2.38	0.41
1:A:817:GLU:CA	1:A:818:ILE:CB	2.99	0.41
1:A:291:THR:C	1:A:293:ASP:N	2.73	0.41
1:A:636:ASP:CG	1:A:636:ASP:O	2.59	0.41
1:A:350:THR:CG2	1:A:350:THR:O	2.69	0.41
1:A:772:ARG:O	1:A:774:ASP:N	2.54	0.40
2:B:506:CYS:N	2:B:512:GLU:OE2	2.54	0.40
2:B:605:GLN:O	2:B:609:GLY:CA	2.70	0.40
1:A:438:ASP:OD2	1:A:470:ARG:NH1	2.55	0.40
1:A:161:GLU:O	1:A:161:GLU:CG	2.67	0.40
1:A:299:ARG:NH1	1:A:299:ARG:CG	2.84	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	Distance(Å)	Clash(Å)
1:A:290:SER:OG	2:B:438:ASP:O[2_454]	2.02	0.18

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	847/904 (94%)	757 (89%)	72 (8%)	18 (2%)	11	48
2	B	337/343 (98%)	311 (92%)	26 (8%)	0	100	100
All	All	1184/1247 (95%)	1068 (90%)	98 (8%)	18 (2%)	15	57

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	55	VAL
1	A	56	THR

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Mol	Chain	Res	Type
1	A	58	LEU
1	A	800	PRO
1	A	818	ILE
1	A	880	VAL
1	A	240	VAL
1	A	292	ARG
1	A	802	GLY
1	A	803	LYS
1	A	755	TRP
1	A	799	GLN
1	A	858	LYS
1	A	89	VAL
1	A	230	ILE
1	A	894	VAL
1	A	303	ASP

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	662/741 (89%)	530 (80%)	132 (20%)	2	8
2	B	271/292 (93%)	233 (86%)	38 (14%)	5	21
All	All	933/1033 (90%)	763 (82%)	170 (18%)	2	10

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	56	THR
1	A	61	LEU
1	A	63	LYS
1	A	65	SER
1	A	66	ASP
1	A	68	LEU
1	A	75	ASN
1	A	76	ILE
1	A	79	LEU

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Mol	Chain	Res	Type
1	A	81	ARG
1	A	83	ASP
1	A	89	VAL
1	A	91	GLN
1	A	106	LYS
1	A	109	VAL
1	A	112	THR
1	A	120	GLN
1	A	122	TYR
1	A	123	THR
1	A	132	ARG
1	A	141	ASN
1	A	143	ILE
1	A	151	VAL
1	A	157	SER
1	A	158	ASN
1	A	162	GLN
1	A	179	ASP
1	A	180	ASP
1	A	181	VAL
1	A	182	ILE
1	A	186	ARG
1	A	187	GLN
1	A	190	ILE
1	A	197	SER
1	A	203	LEU
1	A	204	THR
1	A	207	ILE
1	A	209	LEU
1	A	220	LEU
1	A	226	ARG
1	A	240	VAL
1	A	243	PHE
1	A	250	GLU
1	A	260	VAL
1	A	273	LYS
1	A	275	ASN
1	A	280	VAL
1	A	290	SER
1	A	291	THR
1	A	299	ARG
1	A	301	LEU

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Mol	Chain	Res	Type
1	A	309	SER
1	A	318	PHE
1	A	320	PHE
1	A	344	THR
1	A	349	LEU
1	A	350	THR
1	A	379	LEU
1	A	395	THR
1	A	402	THR
1	A	407	ARG
1	A	412	TYR
1	A	419	LYS
1	A	428	LEU
1	A	429	SER
1	A	439	ASN
1	A	441	PHE
1	A	444	THR
1	A	455	CYS
1	A	460	ASP
1	A	464	SER
1	A	478	ARG
1	A	495	HIS
1	A	498	SER
1	A	499	VAL
1	A	508	SER
1	A	510	LEU
1	A	515	TYR
1	A	524	TYR
1	A	535	LYS
1	A	550	THR
1	A	553	ARG
1	A	556	VAL
1	A	557	VAL
1	A	558	THR
1	A	566	ASN
1	A	567	ASN
1	A	575	ARG
1	A	583	TYR
1	A	588	ASP
1	A	597	ASP
1	A	603	ARG
1	A	620	THR

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Mol	Chain	Res	Type
1	A	622	ARG
1	A	625	SER
1	A	636	ASP
1	A	638	LEU
1	A	670	ILE
1	A	678	LYS
1	A	683	VAL
1	A	688	PHE
1	A	708	TYR
1	A	712	ILE
1	A	713	LYS
1	A	716	LYS
1	A	717	GLU
1	A	722	ASP
1	A	766	VAL
1	A	771	LYS
1	A	772	ARG
1	A	778	ILE
1	A	790	ARG
1	A	814	LYS
1	A	818	ILE
1	A	819	THR
1	A	842	THR
1	A	843	ARG
1	A	848	VAL
1	A	855	THR
1	A	856	VAL
1	A	860	PHE
1	A	861	THR
1	A	871	ASN
1	A	878	GLU
1	A	879	ASN
1	A	892	LYS
1	A	894	VAL
1	A	896	VAL
1	A	899	ARG
1	A	906	ASN
1	A	912	GLU
2	B	347	LEU
2	B	366	ILE
2	B	369	VAL
2	B	374	THR

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Mol	Chain	Res	Type
2	B	391	LEU
2	B	407	VAL
2	B	417	ASN
2	B	421	THR
2	B	444	LEU
2	B	474	CYS
2	B	509	ASN
2	B	525	VAL
2	B	552	LYS
2	B	554	LEU
2	B	556	GLU
2	B	562	LEU
2	B	577	CYS
2	B	579	LEU
2	B	581	ARG
2	B	588	VAL
2	B	590	ARG
2	B	593	LYS
2	B	596	CYS
2	B	601	LEU
2	B	604	GLN
2	B	611	ASN
2	B	612	VAL
2	B	613	THR
2	B	616	SER
2	B	629	LEU
2	B	630	LEU
2	B	632	ARG
2	B	641	LEU
2	B	645	ASN
2	B	648	GLU
2	B	657	LYS
2	B	667	THR
2	B	674	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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	853/904 (94%)	-0.18	1 (0%) 93 70	24, 73, 122, 160	0
2	B	339/343 (98%)	-0.26	0 100 100	31, 69, 112, 126	0
All	All	1192/1247 (95%)	-0.20	1 (0%) 93 70	24, 72, 118, 160	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	621	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

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.