



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:56 PM UTC

PDB ID : 4B7O / pdb_00004b7o
Title : THE FrpB IRON TRANSPORTER FROM NEISSERIA MENINGITIDIS
(F5-1 VARIANT) APOPROTEIN FORM
Authors : Saleem, M.; Prince, S.M.; Derrick, J.P.
Deposited on : 2012-08-21
Resolution : 2.32 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

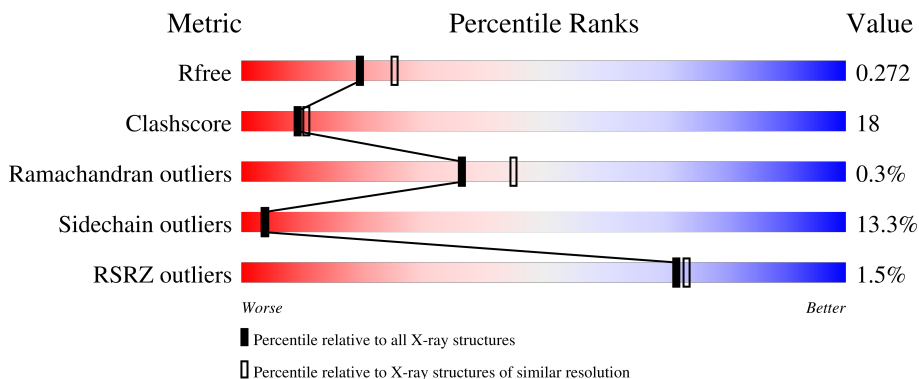
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	745	56% 25% 6% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5182 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 IRON-REGULATED OUTER MEMBRANE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	0
			5103	3197	922	979	5			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q841A2
A	2	HIS	-	expression tag	UNP Q841A2
A	3	HIS	-	expression tag	UNP Q841A2
A	4	HIS	-	expression tag	UNP Q841A2
A	5	HIS	-	expression tag	UNP Q841A2
A	6	HIS	-	expression tag	UNP Q841A2
A	7	HIS	-	expression tag	UNP Q841A2
A	8	SER	-	expression tag	UNP Q841A2
A	9	SER	-	expression tag	UNP Q841A2
A	10	GLY	-	expression tag	UNP Q841A2
A	11	LEU	-	expression tag	UNP Q841A2
A	12	VAL	-	expression tag	UNP Q841A2
A	13	PRO	-	expression tag	UNP Q841A2
A	14	ARG	-	expression tag	UNP Q841A2
A	15	GLY	-	expression tag	UNP Q841A2
A	16	SER	-	expression tag	UNP Q841A2
A	17	GLY	-	expression tag	UNP Q841A2
A	18	MET	-	expression tag	UNP Q841A2
A	19	LYS	-	expression tag	UNP Q841A2
A	20	GLU	-	expression tag	UNP Q841A2
A	21	THR	-	expression tag	UNP Q841A2
A	22	ALA	-	expression tag	UNP Q841A2
A	23	ALA	-	expression tag	UNP Q841A2
A	24	ALA	-	expression tag	UNP Q841A2
A	25	LYS	-	expression tag	UNP Q841A2
A	26	PHE	-	expression tag	UNP Q841A2
A	27	GLU	-	expression tag	UNP Q841A2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ARG	-	expression tag	UNP Q841A2
A	29	GLN	-	expression tag	UNP Q841A2
A	30	HIS	-	expression tag	UNP Q841A2
A	31	MET	-	expression tag	UNP Q841A2
A	32	ASP	-	expression tag	UNP Q841A2
A	33	SER	-	expression tag	UNP Q841A2
A	34	PRO	-	expression tag	UNP Q841A2
A	35	ASP	-	expression tag	UNP Q841A2
A	36	LEU	-	expression tag	UNP Q841A2
A	37	GLY	-	expression tag	UNP Q841A2
A	38	THR	-	expression tag	UNP Q841A2
A	39	ASP	-	expression tag	UNP Q841A2
A	40	ASP	-	expression tag	UNP Q841A2
A	41	ASP	-	expression tag	UNP Q841A2
A	42	ASP	-	expression tag	UNP Q841A2
A	43	LYS	-	expression tag	UNP Q841A2
A	44	MET	-	expression tag	UNP Q841A2
A	45	ALA	-	expression tag	UNP Q841A2
A	46	GLU	-	expression tag	UNP Q841A2
A	47	ASN	-	expression tag	UNP Q841A2
A	48	ASN	-	expression tag	UNP Q841A2
A	49	ALA	-	expression tag	UNP Q841A2
A	50	LYS	-	expression tag	UNP Q841A2
A	51	VAL	-	expression tag	UNP Q841A2
A	724	GLN	-	expression tag	UNP Q841A2
A	725	ARG	-	expression tag	UNP Q841A2
A	726	TRP	-	expression tag	UNP Q841A2
A	727	THR	-	expression tag	UNP Q841A2
A	728	ASN	-	expression tag	UNP Q841A2
A	729	THR	-	expression tag	UNP Q841A2
A	730	LEU	-	expression tag	UNP Q841A2
A	731	PRO	-	expression tag	UNP Q841A2
A	732	GLY	-	expression tag	UNP Q841A2
A	733	VAL	-	expression tag	UNP Q841A2
A	734	GLY	-	expression tag	UNP Q841A2
A	735	ARG	-	expression tag	UNP Q841A2
A	736	ASP	-	expression tag	UNP Q841A2
A	737	VAL	-	expression tag	UNP Q841A2
A	738	ARG	-	expression tag	UNP Q841A2
A	739	LEU	-	expression tag	UNP Q841A2
A	740	GLY	-	expression tag	UNP Q841A2
A	741	VAL	-	expression tag	UNP Q841A2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	742	ASN	-	expression tag	UNP Q841A2
A	743	TYR	-	expression tag	UNP Q841A2
A	744	LYS	-	expression tag	UNP Q841A2
A	745	PHE	-	expression tag	UNP Q841A2
A	272	GLU	LYS	SEE REMARK 999	UNP Q841A2
A	302	PRO	SER	SEE REMARK 999	UNP Q841A2
A	638	ALA	THR	SEE REMARK 999	UNP Q841A2

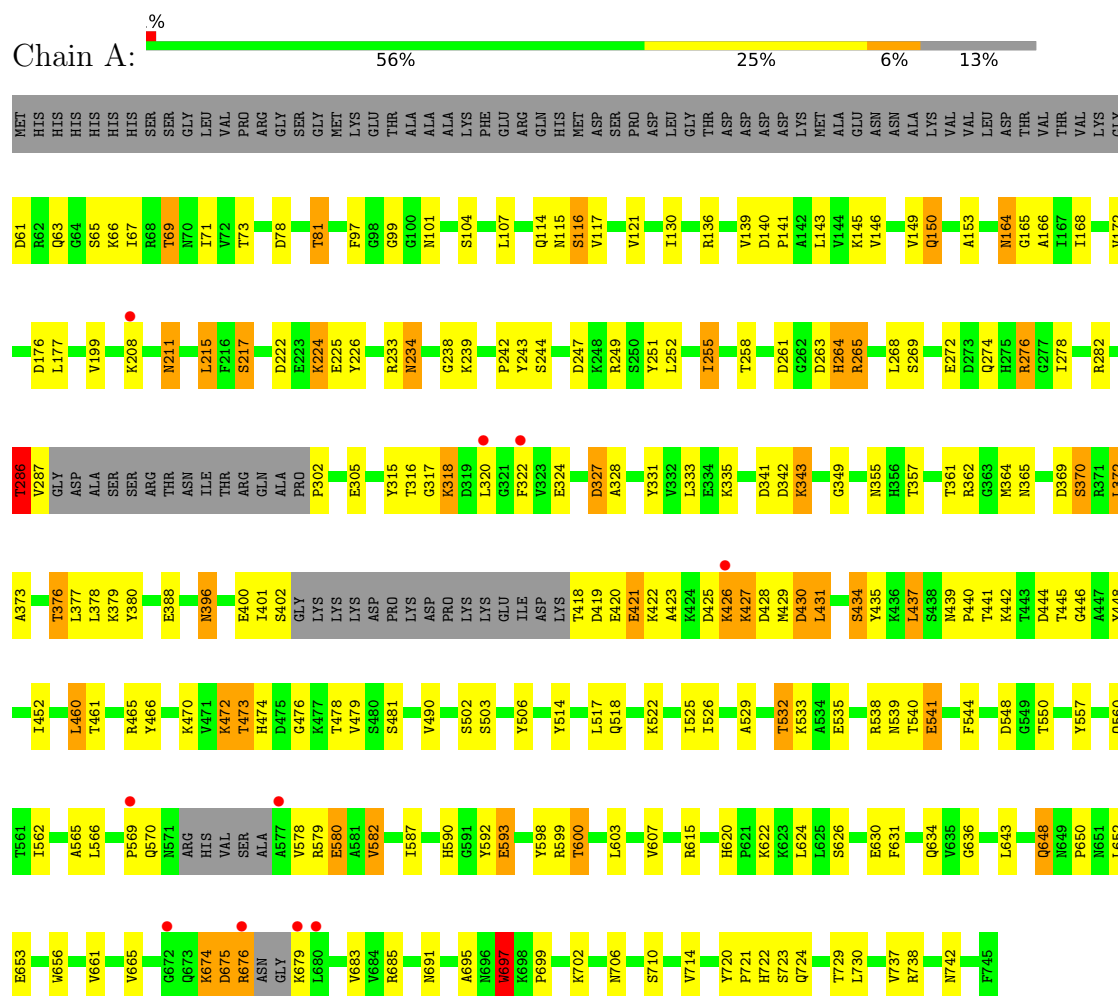
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	79	Total O 79 79	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: IRON-REGULATED OUTER MEMBRANE PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.21Å 79.10Å 74.75Å 90.00° 97.58° 90.00°	Depositor
Resolution (Å)	37.05 – 2.32 37.05 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.0 (37.05-2.32) 98.0 (37.05-2.32)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.233 , 0.281 0.228 , 0.272	Depositor DCC
R_{free} test set	2172 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 22.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5182	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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	1.22	8/5210 (0.2%)	1.23	17/7027 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	SER	N-CA	-6.08	1.38	1.45
1	A	620	HIS	CG-CD2	5.77	1.42	1.35
1	A	697	TRP	CD2-CE2	5.39	1.50	1.41
1	A	331	TYR	N-CA	-5.19	1.39	1.45
1	A	264	HIS	CA-C	-5.09	1.46	1.52
1	A	361	THR	CA-C	-5.03	1.46	1.52
1	A	166	ALA	N-CA	-5.01	1.40	1.46
1	A	722	HIS	CA-C	-5.01	1.45	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	GLU	N-CA-C	7.10	120.23	109.23
1	A	130	ILE	N-CA-C	6.49	116.52	110.42
1	A	222	ASP	CA-C-N	-6.47	114.06	123.00
1	A	222	ASP	C-N-CA	-6.47	114.06	123.00
1	A	164	ASN	CA-C-N	-6.43	112.78	122.04
1	A	164	ASN	C-N-CA	-6.43	112.78	122.04
1	A	636	GLY	N-CA-C	-6.04	104.48	112.82
1	A	697	TRP	CA-CB-CG	5.95	124.89	113.60
1	A	720	TYR	CA-C-N	5.50	125.81	119.92
1	A	720	TYR	C-N-CA	5.50	125.81	119.92
1	A	317	GLY	N-CA-C	5.48	120.47	110.71
1	A	578	VAL	N-CA-C	-5.30	99.53	107.37
1	A	683	VAL	N-CA-C	5.15	115.89	108.93
1	A	286	THR	CB-CA-C	-5.12	101.57	112.63
1	A	723	SER	CB-CA-C	-5.07	104.73	111.88
1	A	226	TYR	CA-C-N	-5.00	115.68	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	TYR	C-N-CA	-5.00	115.68	122.93

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	5103	0	4945	182	0
2	A	79	0	0	22	0
All	All	5182	0	4945	182	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 18.

All (182) 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:615:ARG:HH12	1:A:634:GLN:NE2	1.38	1.19
1:A:316:THR:HB	2:A:2041:HOH:O	1.40	1.18
1:A:427:LYS:HB2	2:A:2052:HOH:O	1.49	1.10
1:A:265:ARG:HB3	2:A:2041:HOH:O	1.56	1.06
1:A:81:THR:HG21	1:A:710:SER:OG	1.55	1.05
1:A:211:ASN:HD22	1:A:211:ASN:N	1.56	1.03
1:A:419:ASP:HB3	1:A:422:LYS:HE2	1.41	1.02
1:A:615:ARG:HH12	1:A:634:GLN:HE21	1.06	1.00
1:A:656:TRP:HE1	1:A:691:ASN:HD22	1.07	0.98
1:A:706:ASN:HD22	1:A:742:ASN:HD21	1.05	0.96
1:A:211:ASN:H	1:A:211:ASN:ND2	1.61	0.91
1:A:582:VAL:HG12	2:A:2059:HOH:O	1.71	0.89
1:A:71:ILE:CD1	1:A:149:VAL:HG23	2.03	0.88
1:A:599:ARG:HD2	2:A:2063:HOH:O	1.72	0.87
1:A:265:ARG:HH11	1:A:265:ARG:HG3	1.38	0.87
1:A:615:ARG:NH1	1:A:634:GLN:NE2	2.22	0.86
1:A:603:LEU:HD11	1:A:643:LEU:HD11	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PRO:HD2	1:A:286:THR:HG21	1.57	0.85
1:A:145:LYS:HD3	1:A:176:ASP:OD2	1.76	0.85
1:A:287:VAL:C	2:A:2044:HOH:O	2.20	0.83
1:A:615:ARG:NH1	1:A:634:GLN:HE21	1.74	0.83
1:A:472:LYS:HE2	1:A:473:THR:O	1.79	0.82
1:A:211:ASN:N	1:A:211:ASN:ND2	2.17	0.81
1:A:478:THR:O	1:A:479:VAL:HG23	1.83	0.78
1:A:150:GLN:O	1:A:165:GLY:HA3	1.84	0.77
1:A:99:GLY:H	1:A:724:GLN:HE22	1.32	0.76
1:A:656:TRP:HE1	1:A:691:ASN:ND2	1.81	0.76
1:A:570:GLN:CD	1:A:582:VAL:HG11	2.10	0.76
1:A:211:ASN:HD22	1:A:211:ASN:H	0.82	0.74
1:A:99:GLY:H	1:A:724:GLN:NE2	1.86	0.73
1:A:341:ASP:OD2	1:A:343:LYS:HE3	1.89	0.73
1:A:373:ALA:HB3	1:A:376:THR:CG2	2.18	0.72
1:A:71:ILE:HD12	1:A:149:VAL:HG23	1.71	0.72
1:A:460:LEU:HD23	1:A:490:VAL:HG12	1.71	0.72
1:A:242:PRO:CD	1:A:286:THR:HG21	2.19	0.71
1:A:440:PRO:HG3	1:A:474:HIS:HB3	1.73	0.70
1:A:373:ALA:HB3	1:A:376:THR:HG23	1.73	0.69
1:A:518:GLN:NE2	2:A:2057:HOH:O	1.61	0.69
1:A:81:THR:HG21	1:A:710:SER:HG	1.54	0.69
1:A:116:SER:HB2	1:A:164:ASN:HD22	1.58	0.69
1:A:691:ASN:O	1:A:714:VAL:HG23	1.93	0.69
1:A:208:LYS:NZ	2:A:2034:HOH:O	2.26	0.68
1:A:656:TRP:NE1	1:A:691:ASN:HD22	1.87	0.67
1:A:421:GLU:C	1:A:421:GLU:OE1	2.37	0.67
1:A:242:PRO:O	1:A:286:THR:CG2	2.43	0.67
1:A:472:LYS:CE	1:A:473:THR:O	2.43	0.66
1:A:599:ARG:CD	2:A:2063:HOH:O	2.35	0.65
1:A:603:LEU:HD11	1:A:643:LEU:CD1	2.25	0.65
1:A:535:GLU:HG2	1:A:565:ALA:HA	1.78	0.65
1:A:242:PRO:O	1:A:286:THR:HG23	1.96	0.65
1:A:255:ILE:CD1	1:A:268:LEU:HB3	2.27	0.64
1:A:265:ARG:HH11	1:A:265:ARG:CG	2.10	0.64
1:A:234:ASN:HB2	1:A:238:GLY:N	2.13	0.64
1:A:255:ILE:HD12	1:A:268:LEU:HB3	1.80	0.63
1:A:569:PRO:HB2	1:A:579:ARG:HB3	1.80	0.62
1:A:63:GLN:NE2	1:A:66:LYS:HD3	2.14	0.62
1:A:472:LYS:HE3	1:A:476:GLY:HA2	1.80	0.62
1:A:461:THR:HG22	2:A:2053:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LYS:HB3	1:A:172:VAL:HA	1.83	0.61
1:A:369:ASP:OD1	1:A:379:LYS:HG2	2.01	0.60
1:A:177:LEU:HD12	1:A:215:LEU:HD12	1.83	0.59
1:A:272:GLU:CD	2:A:2040:HOH:O	2.45	0.59
1:A:478:THR:O	1:A:479:VAL:CG2	2.50	0.59
1:A:478:THR:HG22	1:A:479:VAL:N	2.17	0.59
1:A:529:ALA:HA	1:A:580:GLU:OE1	2.03	0.58
1:A:101:ASN:O	1:A:104:SER:HB2	2.04	0.58
1:A:247:ASP:OD2	1:A:249:ARG:NH2	2.37	0.58
1:A:529:ALA:O	1:A:532:THR:HG23	2.03	0.58
1:A:116:SER:CB	1:A:164:ASN:HD22	2.16	0.57
1:A:264:HIS:HD2	1:A:315:TYR:OH	1.87	0.57
1:A:426:LYS:HB3	1:A:426:LYS:HZ3	1.70	0.57
1:A:372:LEU:HD21	1:A:378:LEU:HD22	1.86	0.57
1:A:650:PRO:HB2	1:A:697:TRP:CZ3	2.39	0.57
1:A:265:ARG:HG3	1:A:265:ARG:NH1	2.17	0.57
1:A:430:ASP:O	1:A:434:SER:OG	2.23	0.56
1:A:648:GLN:HG3	2:A:2070:HOH:O	2.05	0.56
1:A:78:ASP:HB3	1:A:706:ASN:ND2	2.21	0.56
1:A:177:LEU:HD12	1:A:215:LEU:CD1	2.35	0.56
1:A:535:GLU:HG3	1:A:566:LEU:HD12	1.88	0.56
1:A:115:ASN:HB2	1:A:630:GLU:HG2	1.88	0.55
1:A:234:ASN:HD22	1:A:238:GLY:HA3	1.71	0.55
1:A:71:ILE:HD11	1:A:149:VAL:HG23	1.86	0.55
1:A:65:SER:CB	1:A:593:GLU:HG3	2.37	0.55
1:A:706:ASN:HD22	1:A:742:ASN:ND2	1.88	0.54
1:A:61:ASP:OD1	1:A:69:THR:HG23	2.07	0.54
1:A:276:ARG:HB3	1:A:305:GLU:HG2	1.88	0.54
1:A:562:ILE:HB	1:A:587:ILE:HB	1.90	0.54
1:A:324:GLU:HB2	2:A:2046:HOH:O	2.08	0.53
1:A:421:GLU:OE1	1:A:421:GLU:O	2.26	0.53
1:A:150:GLN:O	1:A:165:GLY:CA	2.56	0.53
1:A:328:ALA:HA	1:A:365:ASN:O	2.09	0.53
1:A:428:ASP:O	1:A:431:LEU:N	2.41	0.53
1:A:396:ASN:CG	1:A:437:LEU:HD22	2.34	0.53
1:A:622:LYS:O	1:A:624:LEU:HG	2.10	0.52
1:A:264:HIS:CD2	1:A:315:TYR:OH	2.62	0.52
1:A:265:ARG:CG	1:A:265:ARG:NH1	2.71	0.52
1:A:65:SER:HB3	1:A:593:GLU:HG3	1.91	0.52
1:A:435:TYR:CD2	1:A:525:ILE:HG13	2.46	0.51
1:A:526:ILE:HD11	1:A:579:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:THR:CG2	1:A:479:VAL:N	2.73	0.51
1:A:81:THR:HG23	1:A:738:ARG:HD3	1.93	0.51
1:A:615:ARG:HH12	1:A:634:GLN:HE22	1.45	0.51
1:A:278:ILE:N	1:A:278:ILE:HD13	2.26	0.51
1:A:548:ASP:OD1	1:A:548:ASP:C	2.52	0.51
1:A:282:ARG:NH1	2:A:2043:HOH:O	2.31	0.50
1:A:598:TYR:CE2	1:A:600:THR:HG22	2.46	0.50
1:A:448:TYR:HB3	1:A:465:ARG:HG2	1.93	0.50
1:A:153:ALA:HB3	1:A:539:ASN:HB3	1.93	0.50
1:A:514:TYR:CD2	1:A:526:ILE:HG13	2.47	0.50
1:A:685:ARG:NH2	1:A:724:GLN:O	2.44	0.50
1:A:388:GLU:HG3	1:A:441:THR:HG22	1.94	0.50
1:A:302:PRO:HD2	2:A:2045:HOH:O	2.11	0.49
1:A:274:GLN:OE1	1:A:276:ARG:NH1	2.45	0.49
1:A:322:PHE:O	1:A:370:SER:HB3	2.11	0.49
1:A:529:ALA:HB3	1:A:532:THR:CG2	2.42	0.49
1:A:258:THR:HG23	1:A:264:HIS:O	2.12	0.49
1:A:506:TYR:OH	1:A:538:ARG:HD3	2.12	0.49
1:A:67:ILE:HG12	1:A:150:GLN:HG3	1.95	0.49
1:A:653:GLU:O	1:A:695:ALA:HA	2.13	0.48
1:A:569:PRO:HA	1:A:580:GLU:O	2.14	0.48
1:A:380:TYR:CD1	1:A:380:TYR:N	2.82	0.47
1:A:675:ASP:OD1	1:A:676:ARG:N	2.48	0.47
1:A:590:HIS:HE1	2:A:2060:HOH:O	1.96	0.47
1:A:143:LEU:O	1:A:172:VAL:HG12	2.15	0.47
1:A:234:ASN:HD22	1:A:238:GLY:CA	2.27	0.46
1:A:243:TYR:HE2	1:A:287:VAL:HG21	1.80	0.46
1:A:243:TYR:HE2	1:A:287:VAL:CG2	2.29	0.46
1:A:263:ASP:HA	1:A:318:LYS:HD2	1.97	0.46
1:A:107:LEU:C	1:A:107:LEU:HD23	2.39	0.46
1:A:615:ARG:CZ	1:A:634:GLN:HE21	2.29	0.46
1:A:421:GLU:HG2	2:A:2051:HOH:O	2.15	0.46
1:A:99:GLY:N	1:A:721:PRO:HG2	2.31	0.46
1:A:697:TRP:CH2	1:A:699:PRO:HA	2.50	0.46
1:A:217:SER:O	1:A:251:TYR:HA	2.17	0.45
1:A:242:PRO:N	1:A:286:THR:HG21	2.31	0.45
1:A:517:LEU:HG	1:A:517:LEU:O	2.15	0.45
1:A:569:PRO:HB3	1:A:580:GLU:C	2.41	0.45
1:A:626:SER:HB3	1:A:631:PHE:CE2	2.51	0.45
1:A:423:ALA:HB2	2:A:2051:HOH:O	2.16	0.45
1:A:140:ASP:HA	1:A:141:PRO:HD2	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:HD11	1:A:268:LEU:HB3	1.98	0.45
1:A:71:ILE:CD1	1:A:149:VAL:CG2	2.87	0.45
1:A:439:ASN:HA	1:A:440:PRO:HD3	1.84	0.45
1:A:242:PRO:HB2	1:A:286:THR:HG22	1.99	0.44
1:A:590:HIS:CE1	2:A:2060:HOH:O	2.70	0.44
1:A:396:ASN:OD1	1:A:396:ASN:N	2.47	0.44
1:A:674:LYS:NZ	1:A:674:LYS:HB3	2.32	0.44
1:A:349:GLY:HA2	1:A:522:LYS:HD3	2.00	0.44
1:A:401:ILE:HG21	1:A:425:ASP:CG	2.42	0.44
1:A:225:GLU:HG2	1:A:244:SER:H	1.82	0.44
1:A:423:ALA:CB	2:A:2051:HOH:O	2.65	0.44
1:A:615:ARG:HD3	1:A:615:ARG:HA	1.81	0.44
1:A:225:GLU:OE2	1:A:243:TYR:N	2.35	0.43
1:A:478:THR:C	1:A:479:VAL:HG23	2.43	0.43
1:A:97:PHE:CE2	1:A:107:LEU:HD12	2.53	0.43
1:A:369:ASP:HB3	1:A:377:LEU:HD11	2.00	0.43
1:A:143:LEU:HD22	1:A:252:LEU:HB2	2.00	0.43
1:A:327:ASP:O	1:A:327:ASP:OD1	2.36	0.43
1:A:81:THR:CG2	1:A:738:ARG:HD3	2.49	0.43
1:A:557:TYR:CD2	1:A:592:TYR:HB3	2.52	0.43
1:A:114:GLN:HB3	1:A:136:ARG:HD2	2.01	0.43
1:A:233:ARG:HD3	1:A:233:ARG:HA	1.78	0.42
1:A:211:ASN:CB	1:A:258:THR:O	2.68	0.42
1:A:446:GLY:HA2	1:A:466:TYR:O	2.19	0.42
1:A:139:VAL:HG22	1:A:140:ASP:N	2.35	0.42
1:A:255:ILE:HD11	1:A:268:LEU:HD23	2.00	0.42
1:A:224:LYS:N	1:A:224:LYS:HD3	2.33	0.42
1:A:442:LYS:HE3	1:A:444:ASP:OD2	2.19	0.42
1:A:652:LEU:HD12	1:A:697:TRP:HB2	2.01	0.42
1:A:251:TYR:HE2	2:A:2040:HOH:O	2.01	0.42
1:A:342:ASP:OD2	1:A:355:ASN:HB3	2.20	0.41
1:A:423:ALA:HA	1:A:426:LYS:NZ	2.35	0.41
1:A:376:THR:HA	1:A:452:ILE:O	2.19	0.41
1:A:435:TYR:HB3	1:A:437:LEU:HD13	2.03	0.41
1:A:316:THR:CB	2:A:2041:HOH:O	2.24	0.41
1:A:502:SER:HA	1:A:541:GLU:O	2.20	0.41
1:A:263:ASP:HA	1:A:318:LYS:CD	2.51	0.41
1:A:579:ARG:HE	1:A:579:ARG:HB2	1.55	0.41
1:A:526:ILE:CD1	1:A:579:ARG:HH21	2.35	0.40
1:A:544:PHE:CD1	1:A:544:PHE:C	3.00	0.40
1:A:211:ASN:HB3	1:A:258:THR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:THR:OG1	1:A:730:LEU:N	2.54	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	639/745 (86%)	613 (96%)	24 (4%)	2 (0%)	36 45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	675	ASP

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	535/615 (87%)	464 (87%)	71 (13%)	4 4

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	THR

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Mol	Chain	Res	Type
1	A	73	THR
1	A	81	THR
1	A	116	SER
1	A	117	VAL
1	A	121	VAL
1	A	146	VAL
1	A	150	GLN
1	A	168	ILE
1	A	199	VAL
1	A	211	ASN
1	A	215	LEU
1	A	217	SER
1	A	224	LYS
1	A	239	LYS
1	A	255	ILE
1	A	261	ASP
1	A	265	ARG
1	A	276	ARG
1	A	286	THR
1	A	318	LYS
1	A	320	LEU
1	A	327	ASP
1	A	333	LEU
1	A	335	LYS
1	A	343	LYS
1	A	357	THR
1	A	362	ARG
1	A	364	MET
1	A	370	SER
1	A	372	LEU
1	A	376	THR
1	A	396	ASN
1	A	400	GLU
1	A	402	SER
1	A	418	THR
1	A	420	GLU
1	A	421	GLU
1	A	426	LYS
1	A	427	LYS
1	A	429	MET
1	A	430	ASP
1	A	431	LEU

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Mol	Chain	Res	Type
1	A	434	SER
1	A	437	LEU
1	A	445	THR
1	A	460	LEU
1	A	470	LYS
1	A	472	LYS
1	A	473	THR
1	A	481	SER
1	A	503	SER
1	A	532	THR
1	A	533	LYS
1	A	540	THR
1	A	550	THR
1	A	560	GLN
1	A	580	GLU
1	A	582	VAL
1	A	593	GLU
1	A	600	THR
1	A	607	VAL
1	A	648	GLN
1	A	661	VAL
1	A	665	VAL
1	A	674	LYS
1	A	676	ARG
1	A	679	LYS
1	A	697	TRP
1	A	702	LYS
1	A	737	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	164	ASN
1	A	175	GLN
1	A	211	ASN
1	A	234	ASN
1	A	264	HIS
1	A	308	GLN
1	A	386	HIS
1	A	387	GLN
1	A	560	GLN

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Mol	Chain	Res	Type
1	A	611	HIS
1	A	634	GLN
1	A	691	ASN
1	A	724	GLN
1	A	728	ASN
1	A	742	ASN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	649/745 (87%)	0.16	10 (1%) 72 73	29, 43, 61, 88	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	577	ALA	4.3
1	A	569	PRO	2.7
1	A	676	ARG	2.6
1	A	208	LYS	2.4
1	A	672	GLY	2.3
1	A	679	LYS	2.2
1	A	322	PHE	2.0
1	A	320	LEU	2.0
1	A	680	LEU	2.0
1	A	426	LYS	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.