



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:38 AM UTC

PDB ID : 4AIQ / pdb_00004aiq
Title : The FrpB iron transporter from *Neisseria meningitidis* (F5-1 variant)
Authors : Saleem, M.; Prince, S.M.; Derrick, J.P.
Deposited on : 2012-02-11
Resolution : 2.60 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

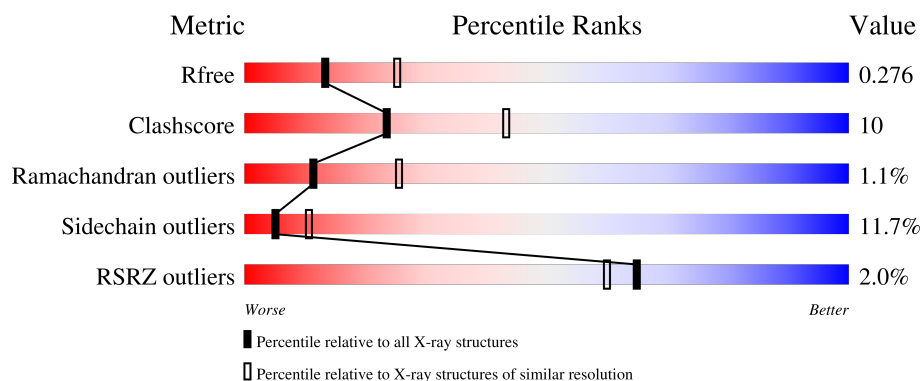
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	745	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5218 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 FERRIC ENTEROBACTIN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	0	0	0
			5168	3235	938	990	5			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP F0N0E1
A	2	HIS	-	expression tag	UNP F0N0E1
A	3	HIS	-	expression tag	UNP F0N0E1
A	4	HIS	-	expression tag	UNP F0N0E1
A	5	HIS	-	expression tag	UNP F0N0E1
A	6	HIS	-	expression tag	UNP F0N0E1
A	7	HIS	-	expression tag	UNP F0N0E1
A	8	SER	-	expression tag	UNP F0N0E1
A	9	SER	-	expression tag	UNP F0N0E1
A	10	GLY	-	expression tag	UNP F0N0E1
A	11	LEU	-	expression tag	UNP F0N0E1
A	12	VAL	-	expression tag	UNP F0N0E1
A	13	PRO	-	expression tag	UNP F0N0E1
A	14	ARG	-	expression tag	UNP F0N0E1
A	15	GLY	-	expression tag	UNP F0N0E1
A	16	SER	-	expression tag	UNP F0N0E1
A	17	GLY	-	expression tag	UNP F0N0E1
A	18	MET	-	expression tag	UNP F0N0E1
A	19	LYS	-	expression tag	UNP F0N0E1
A	20	GLU	-	expression tag	UNP F0N0E1
A	21	THR	-	expression tag	UNP F0N0E1
A	22	ALA	-	expression tag	UNP F0N0E1
A	23	ALA	-	expression tag	UNP F0N0E1
A	24	ALA	-	expression tag	UNP F0N0E1
A	25	LYS	-	expression tag	UNP F0N0E1
A	26	PHE	-	expression tag	UNP F0N0E1
A	27	GLU	-	expression tag	UNP F0N0E1

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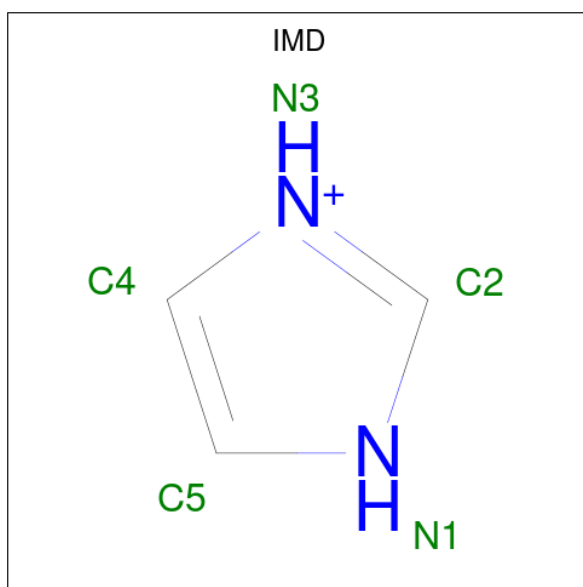
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Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ARG	-	expression tag	UNP F0N0E1
A	29	GLN	-	expression tag	UNP F0N0E1
A	30	HIS	-	expression tag	UNP F0N0E1
A	31	MET	-	expression tag	UNP F0N0E1
A	32	ASP	-	expression tag	UNP F0N0E1
A	33	SER	-	expression tag	UNP F0N0E1
A	34	PRO	-	expression tag	UNP F0N0E1
A	35	ASP	-	expression tag	UNP F0N0E1
A	36	LEU	-	expression tag	UNP F0N0E1
A	37	GLY	-	expression tag	UNP F0N0E1
A	38	THR	-	expression tag	UNP F0N0E1
A	39	ASP	-	expression tag	UNP F0N0E1
A	40	ASP	-	expression tag	UNP F0N0E1
A	41	ASP	-	expression tag	UNP F0N0E1
A	42	ASP	-	expression tag	UNP F0N0E1
A	43	LYS	-	expression tag	UNP F0N0E1
A	44	MET	-	expression tag	UNP F0N0E1
A	272	GLU	LYS	variant	UNP F0N0E1
A	302	PRO	SER	variant	UNP F0N0E1
A	455	LEU	ILE	variant	UNP F0N0E1
A	638	ALA	THR	variant	UNP F0N0E1

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		

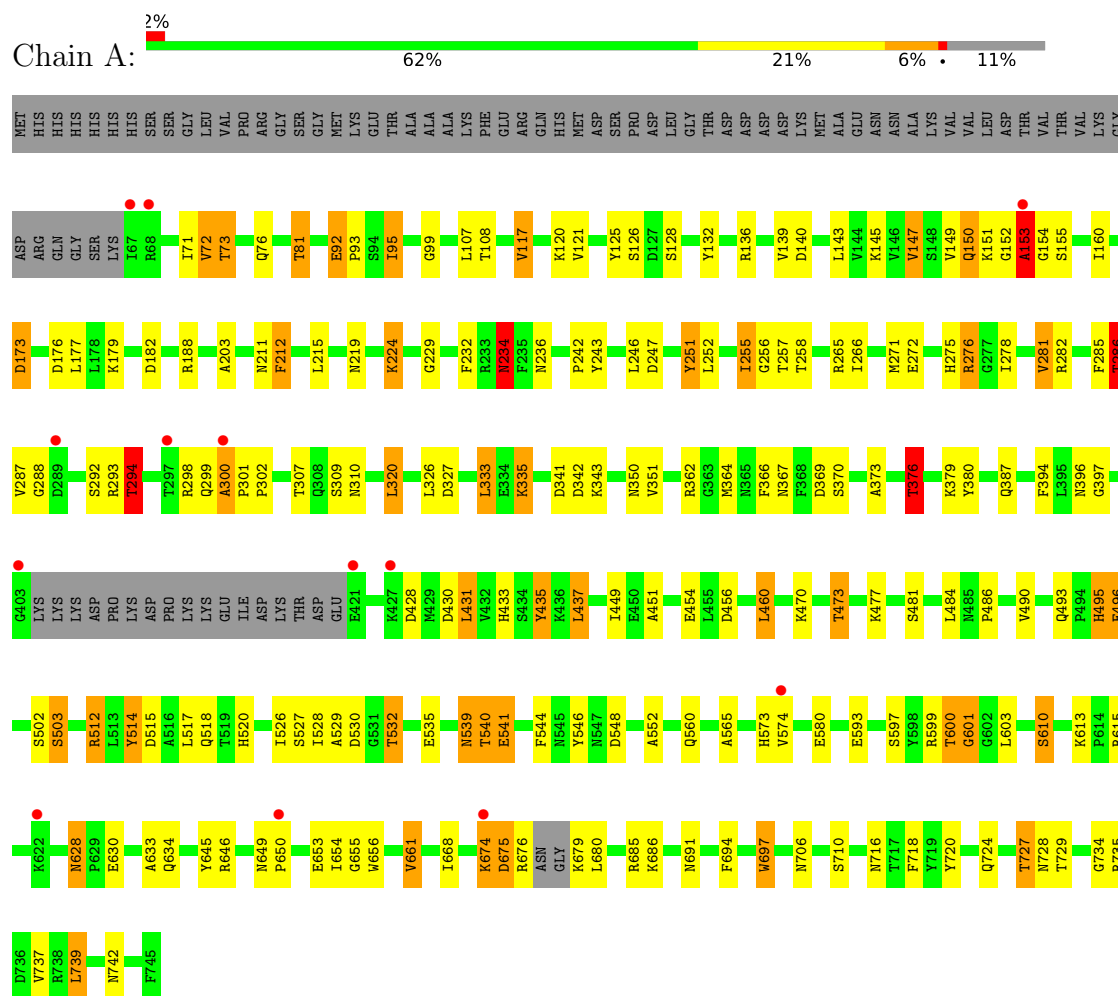
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		

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: FERRIC ENTEROBACTIN RECEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.98Å 78.69Å 73.43Å 90.00° 97.22° 90.00°	Depositor
Resolution (Å)	36.42 – 2.60 36.42 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (36.42-2.60) 97.2 (36.42-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.227 , 0.277 0.223 , 0.276	Depositor DCC
R_{free} test set	1508 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 21.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5218	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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

Bond lengths and bond angles in the following residue types are not validated in this section: FE, IMD

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	1.37	12/5279 (0.2%)	1.36	35/7128 (0.5%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	ILE	CA-CB	7.01	1.61	1.53
1	A	154	GLY	C-O	6.84	1.28	1.23
1	A	503	SER	CA-C	-5.42	1.46	1.52
1	A	300	ALA	C-O	5.41	1.26	1.23
1	A	73	THR	CA-CB	5.29	1.61	1.53
1	A	486	PRO	C-O	-5.29	1.17	1.23
1	A	310	ASN	CA-C	-5.26	1.46	1.52
1	A	335	LYS	CA-C	5.23	1.58	1.52
1	A	173	ASP	CA-C	-5.21	1.46	1.52
1	A	451	ALA	N-CA	5.21	1.52	1.46
1	A	435	TYR	C-O	-5.20	1.17	1.23
1	A	739	LEU	N-CA	-5.00	1.39	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540	THR	CB-CA-C	8.05	125.28	109.35
1	A	351	VAL	N-CA-C	-7.89	99.43	109.30
1	A	628	ASN	CA-C-N	7.60	128.28	119.47
1	A	628	ASN	C-N-CA	7.60	128.28	119.47
1	A	154	GLY	N-CA-C	-7.50	103.90	111.85
1	A	541	GLU	N-CA-C	7.36	120.04	108.79
1	A	160	ILE	N-CA-C	7.35	118.48	109.30
1	A	234	ASN	CB-CA-C	-6.64	97.20	110.42
1	A	697	TRP	CA-CB-CG	6.33	125.62	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	LYS	N-CA-C	-6.13	98.91	108.90
1	A	376	THR	CB-CA-C	5.87	119.48	110.62
1	A	117	VAL	N-CA-C	5.80	116.46	107.99
1	A	294	THR	CB-CA-C	5.62	120.13	111.02
1	A	428	ASP	N-CA-C	5.61	117.07	111.07
1	A	661	VAL	CB-CA-C	5.50	118.77	110.63
1	A	150	GLN	CB-CA-C	-5.48	101.77	110.81
1	A	727	THR	N-CA-C	-5.42	101.64	110.20
1	A	307	THR	N-CA-C	5.41	117.90	108.76
1	A	493	GLN	CA-C-N	-5.35	114.16	119.56
1	A	493	GLN	C-N-CA	-5.35	114.16	119.56
1	A	739	LEU	CA-C-N	5.30	126.49	121.46
1	A	739	LEU	C-N-CA	5.30	126.49	121.46
1	A	147	VAL	CB-CA-C	-5.26	102.66	110.33
1	A	286	THR	CB-CA-C	-5.23	100.02	110.42
1	A	92	GLU	CA-C-N	-5.21	114.29	119.56
1	A	92	GLU	C-N-CA	-5.21	114.29	119.56
1	A	520	HIS	N-CA-C	5.18	117.60	111.33
1	A	72	VAL	CB-CA-C	5.17	118.12	110.77
1	A	573	HIS	N-CA-C	-5.10	101.84	109.79
1	A	72	VAL	N-CA-C	5.05	115.13	107.75
1	A	153	ALA	N-CA-C	-5.05	100.04	110.80
1	A	251	TYR	N-CA-C	5.04	116.84	109.24
1	A	539	ASN	CA-C-N	-5.03	114.58	122.73
1	A	539	ASN	C-N-CA	-5.03	114.58	122.73
1	A	477	LYS	N-CA-C	5.03	117.52	110.23

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	5168	0	5002	104	0
2	A	1	0	0	0	0
3	A	5	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	44	0	0	0	0
All	All	5218	0	5006	104	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 (104) 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:HE21	1.13	0.97
1:A:706:ASN:HD22	1:A:742:ASN:HD21	1.03	0.96
1:A:535:GLU:HG2	1:A:565:ALA:HA	1.57	0.85
1:A:656:TRP:HE1	1:A:691:ASN:HD22	1.26	0.83
1:A:145:LYS:HD3	1:A:176:ASP:OD2	1.79	0.82
1:A:300:ALA:O	1:A:302:PRO:HD3	1.79	0.82
1:A:685:ARG:NH2	1:A:724:GLN:O	2.16	0.77
1:A:706:ASN:HD22	1:A:742:ASN:ND2	1.80	0.76
1:A:706:ASN:ND2	1:A:742:ASN:HD21	1.83	0.75
1:A:373:ALA:HB3	1:A:376:THR:HG23	1.69	0.74
1:A:288:GLY:N	1:A:294:THR:HG22	2.03	0.74
1:A:281:VAL:HG12	1:A:282:ARG:HG3	1.71	0.72
1:A:364:MET:HG2	1:A:366:PHE:CE1	2.28	0.68
1:A:288:GLY:H	1:A:294:THR:HG22	1.58	0.68
1:A:656:TRP:HE1	1:A:691:ASN:ND2	1.92	0.67
1:A:495:HIS:ND1	1:A:496:GLU:N	2.42	0.67
1:A:93:PRO:HB2	1:A:610:SER:HB3	1.78	0.66
1:A:242:PRO:O	1:A:286:THR:HG22	1.96	0.65
1:A:460:LEU:HD23	1:A:490:VAL:HG12	1.78	0.65
1:A:373:ALA:HB3	1:A:376:THR:CG2	2.26	0.65
1:A:615:ARG:HH12	1:A:634:GLN:NE2	1.89	0.64
1:A:529:ALA:O	1:A:532:THR:HG23	1.98	0.64
1:A:107:LEU:C	1:A:107:LEU:HD23	2.22	0.64
1:A:615:ARG:NH1	1:A:634:GLN:HE21	1.91	0.63
1:A:242:PRO:HD2	1:A:286:THR:HG21	1.81	0.62
1:A:675:ASP:OD1	1:A:679:LYS:HB3	1.99	0.62
1:A:73:THR:HG22	1:A:76:GLN:OE1	2.00	0.61
1:A:369:ASP:OD1	1:A:379:LYS:HG2	2.01	0.61
1:A:656:TRP:NE1	1:A:691:ASN:HD22	1.97	0.60
1:A:539:ASN:ND2	1:A:560:GLN:HG3	2.18	0.59
1:A:674:LYS:HA	1:A:679:LYS:O	2.02	0.59
1:A:152:GLY:O	1:A:153:ALA:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:HG3	1:A:95:ILE:HG12	1.86	0.58
1:A:99:GLY:H	1:A:724:GLN:NE2	2.01	0.58
1:A:431:LEU:HD22	1:A:435:TYR:CE2	2.40	0.57
1:A:246:LEU:HD22	1:A:275:HIS:HB3	1.88	0.56
1:A:81:THR:HG21	1:A:710:SER:OG	2.06	0.55
1:A:396:ASN:OD1	1:A:396:ASN:N	2.40	0.55
1:A:512:ARG:HH22	1:A:535:GLU:CD	2.15	0.55
1:A:613:LYS:HA	1:A:634:GLN:HE22	1.73	0.54
1:A:309:SER:O	1:A:333:LEU:HD23	2.07	0.54
1:A:343:LYS:O	1:A:350:ASN:HB3	2.08	0.54
1:A:232:PHE:HB2	1:A:718:PHE:CE1	2.43	0.54
1:A:173:ASP:HB2	1:A:176:ASP:OD2	2.07	0.54
1:A:132:TYR:HD2	1:A:628:ASN:ND2	2.07	0.53
1:A:517:LEU:HG	1:A:517:LEU:O	2.09	0.53
1:A:720:TYR:CZ	1:A:728:ASN:HB3	2.44	0.53
1:A:99:GLY:H	1:A:724:GLN:HE22	1.55	0.53
1:A:548:ASP:OD1	1:A:548:ASP:C	2.52	0.53
1:A:247:ASP:HB3	1:A:276:ARG:HG2	1.91	0.52
1:A:326:LEU:HD12	1:A:367:ASN:O	2.09	0.52
1:A:734:GLY:O	1:A:735:ARG:C	2.52	0.52
1:A:243:TYR:CZ	1:A:301:PRO:HG3	2.45	0.52
1:A:151:LYS:NZ	1:A:593:GLU:HG3	2.25	0.51
1:A:107:LEU:HD23	1:A:108:THR:N	2.26	0.51
1:A:380:TYR:CD1	1:A:380:TYR:N	2.80	0.49
1:A:552:ALA:HB3	1:A:597:SER:OG	2.13	0.49
1:A:151:LYS:HZ3	1:A:593:GLU:HG3	1.76	0.49
1:A:514:TYR:CG	1:A:526:ILE:HG21	2.47	0.49
1:A:341:ASP:OD2	1:A:343:LYS:HE3	2.12	0.49
1:A:265:ARG:HH11	1:A:265:ARG:HG3	1.78	0.48
1:A:544:PHE:CD1	1:A:544:PHE:C	2.91	0.48
1:A:212:PHE:HE2	1:A:255:ILE:HG22	1.79	0.48
1:A:473:THR:HG21	1:A:527:SER:HA	1.94	0.47
1:A:292:SER:C	1:A:294:THR:H	2.21	0.47
1:A:431:LEU:HD22	1:A:435:TYR:HE2	1.77	0.47
1:A:234:ASN:HB3	1:A:236:ASN:H	1.80	0.47
1:A:120:LYS:HA	1:A:125:TYR:HB3	1.94	0.47
1:A:152:GLY:O	1:A:153:ALA:CB	2.62	0.47
1:A:286:THR:HB	1:A:287:VAL:H	1.28	0.47
1:A:320:LEU:HD23	1:A:320:LEU:O	2.14	0.47
1:A:546:TYR:OH	1:A:548:ASP:OD2	2.25	0.46
1:A:364:MET:HG2	1:A:366:PHE:HE1	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:SER:OG	1:A:387:GLN:NE2	2.49	0.46
1:A:394:PHE:CD2	1:A:437:LEU:HB3	2.51	0.46
1:A:437:LEU:HD12	1:A:437:LEU:HA	1.76	0.45
1:A:177:LEU:HD12	1:A:215:LEU:CD1	2.46	0.45
1:A:211:ASN:HB2	1:A:258:THR:O	2.17	0.45
1:A:650:PRO:HB2	1:A:697:TRP:CZ3	2.52	0.45
1:A:599:ARG:HA	1:A:603:LEU:O	2.17	0.44
1:A:143:LEU:HD13	1:A:271:MET:SD	2.58	0.44
1:A:229:GLY:HA2	1:A:716:ASN:OD1	2.17	0.44
1:A:139:VAL:HG22	1:A:140:ASP:N	2.33	0.44
1:A:188:ARG:O	1:A:203:ALA:HA	2.17	0.44
1:A:151:LYS:NZ	1:A:593:GLU:CG	2.80	0.44
1:A:136:ARG:NH1	1:A:630:GLU:HG3	2.33	0.43
1:A:252:LEU:HD13	1:A:271:MET:HB2	1.99	0.43
1:A:177:LEU:HD12	1:A:215:LEU:HD11	2.00	0.43
1:A:285:PHE:HB2	1:A:299:GLN:NE2	2.34	0.43
1:A:502:SER:HA	1:A:541:GLU:O	2.19	0.43
1:A:107:LEU:C	1:A:107:LEU:CD2	2.91	0.42
1:A:655:GLY:HA3	1:A:694:PHE:CZ	2.53	0.42
1:A:242:PRO:O	1:A:286:THR:CG2	2.67	0.42
1:A:251:TYR:CE2	1:A:272:GLU:HG3	2.55	0.42
1:A:600:THR:O	1:A:601:GLY:C	2.63	0.42
1:A:727:THR:O	1:A:729:THR:HG23	2.20	0.42
1:A:256:GLY:HA2	1:A:266:ILE:O	2.20	0.42
1:A:224:LYS:HA	1:A:224:LYS:HD2	1.68	0.42
1:A:645:TYR:O	1:A:653:GLU:HA	2.20	0.42
1:A:342:ASP:O	1:A:350:ASN:HA	2.19	0.41
1:A:397:GLY:O	1:A:433:HIS:CD2	2.73	0.41
1:A:685:ARG:O	1:A:686:LYS:C	2.63	0.41
1:A:633:ALA:HA	1:A:668:ILE:CG2	2.51	0.41
1:A:139:VAL:CG2	1:A:140:ASP:N	2.85	0.41

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	654/745 (88%)	615 (94%)	32 (5%)	7 (1%)	11	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ALA
1	A	574	VAL
1	A	601	GLY
1	A	234	ASN
1	A	675	ASP
1	A	293	ARG
1	A	514	TYR

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	540/615 (88%)	477 (88%)	63 (12%)	5	11

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ILE
1	A	72	VAL
1	A	81	THR
1	A	95	ILE
1	A	117	VAL
1	A	121	VAL
1	A	126	SER
1	A	147	VAL
1	A	149	VAL
1	A	150	GLN
1	A	155	SER
1	A	179	LYS

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Mol	Chain	Res	Type
1	A	182	ASP
1	A	212	PHE
1	A	219	ASN
1	A	224	LYS
1	A	255	ILE
1	A	257	THR
1	A	276	ARG
1	A	281	VAL
1	A	286	THR
1	A	294	THR
1	A	298	ARG
1	A	320	LEU
1	A	327	ASP
1	A	333	LEU
1	A	335	LYS
1	A	362	ARG
1	A	370	SER
1	A	376	THR
1	A	430	ASP
1	A	431	LEU
1	A	437	LEU
1	A	449	ILE
1	A	454	GLU
1	A	456	ASP
1	A	460	LEU
1	A	470	LYS
1	A	473	THR
1	A	481	SER
1	A	484	LEU
1	A	495	HIS
1	A	496	GLU
1	A	503	SER
1	A	512	ARG
1	A	515	ASP
1	A	518	GLN
1	A	528	ILE
1	A	530	ASP
1	A	532	THR
1	A	540	THR
1	A	580	GLU
1	A	600	THR
1	A	610	SER

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Mol	Chain	Res	Type
1	A	646	ARG
1	A	649	ASN
1	A	654	ILE
1	A	661	VAL
1	A	674	LYS
1	A	676	ARG
1	A	680	LEU
1	A	737	VAL
1	A	739	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	A	175	GLN
1	A	190	ASN
1	A	211	ASN
1	A	264	HIS
1	A	274	GLN
1	A	375	GLN
1	A	386	HIS
1	A	387	GLN
1	A	392	GLN
1	A	539	ASN
1	A	560	GLN
1	A	570	GLN
1	A	634	GLN
1	A	651	ASN
1	A	691	ASN
1	A	712	ASN
1	A	724	GLN
1	A	742	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	IMD	A	1747	2	5,5,5	1.12	0	5,5,5	0.73	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMD	A	1747	2	-	-	0/1/1/1

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 [i](#)

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 [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	660/745 (88%)	0.05	13 (1%) 65 60	31, 47, 69, 92	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	ALA	4.1
1	A	421	GLU	3.9
1	A	67	ILE	3.7
1	A	300	ALA	3.1
1	A	297	THR	2.7
1	A	289	ASP	2.5
1	A	427	LYS	2.4
1	A	574	VAL	2.4
1	A	674	LYS	2.4
1	A	68	ARG	2.3
1	A	650	PRO	2.3
1	A	403	GLY	2.2
1	A	622	LYS	2.1

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](#)

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($\text{\AA}^2$)	Q<0.9
3	IMD	A	1747	5/5	0.76	0.22	61,61,64,65	0
2	FE	A	1746	1/1	0.99	0.03	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.