



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:40 am BST

PDB ID : 1FEP
Title : FERRIC ENTEROBACTIN RECEPTOR
Authors : Buchanan, S.K.; Smith, B.S.; Ventatramani, L.; Xia, D.; Esser, L.; Palnitkar, M.; Chakraborty, R.; Van Der Helm, D.; Deisenhofer, J.
Deposited on : 1998-11-24
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

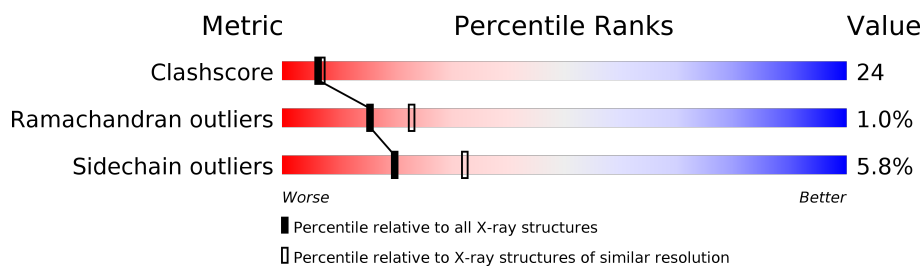
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	724	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5514 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	680	Total	C	N	O	Se	0	0	0
			5300	3308	935	1046	11			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	MSE	MET	MODIFIED RESIDUE	UNP P05825
A	77	MSE	MET	MODIFIED RESIDUE	UNP P05825
A	118	MSE	MET	MODIFIED RESIDUE	UNP P05825
A	346	MSE	MET	MODIFIED RESIDUE	UNP P05825
A	374	MSE	MET	MODIFIED RESIDUE	UNP P05825
A	418	MSE	MET	MODIFIED RESIDUE	UNP P05825
A	460	MSE	MET	MODIFIED RESIDUE	UNP P05825
A	579	MSE	MET	MODIFIED RESIDUE	UNP P05825
A	587	MSE	MET	MODIFIED RESIDUE	UNP P05825
A	621	MSE	MET	MODIFIED RESIDUE	UNP P05825
A	718	MSE	MET	MODIFIED RESIDUE	UNP P05825

- Molecule 2 is water.

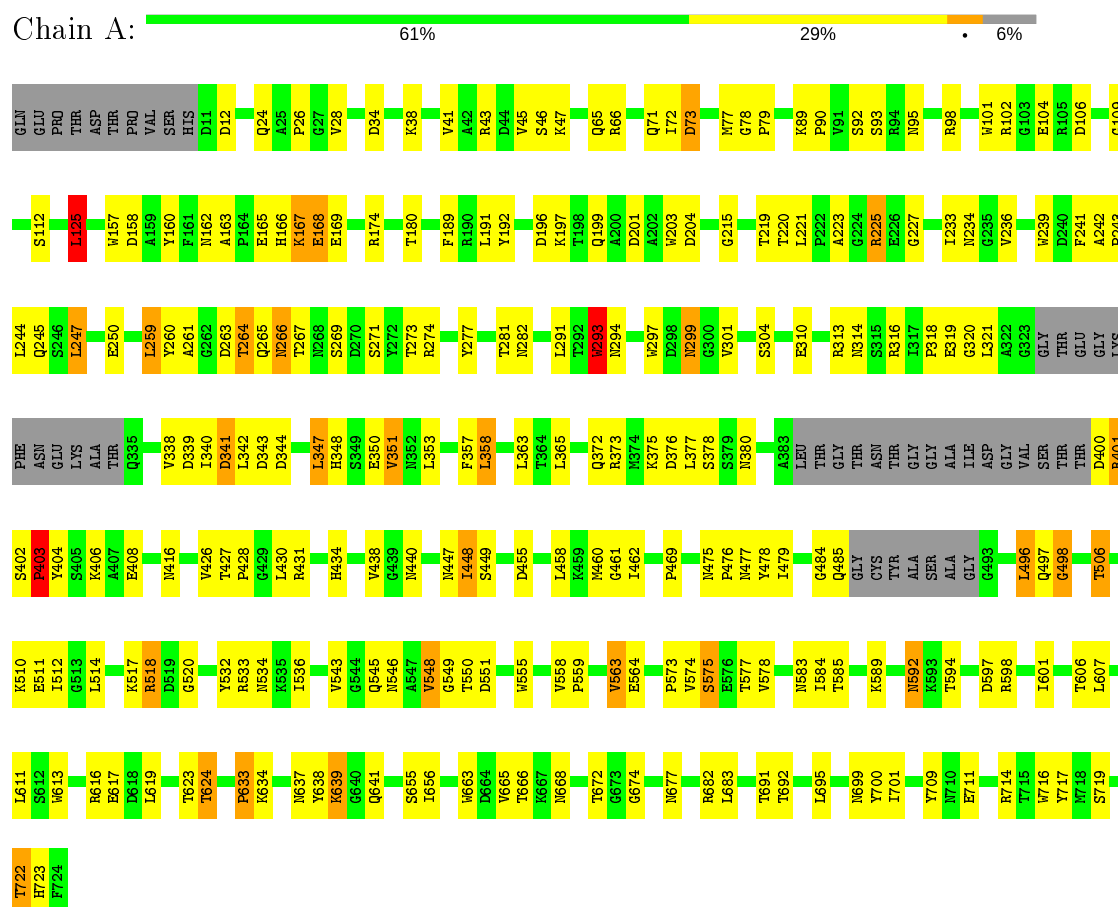
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	214	Total	O	0	0
			214	214		

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

• Molecule 1: FERRIC ENTEROBACTIN RECEPTOR



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	112.30 Å 127.60 Å 135.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	96.9 (20.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.3C	Depositor
R, R_{free}	0.236 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5514	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

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	0.89	1/5406 (0.0%)	1.03	13/7333 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TYR	CE2-CZ	5.07	1.45	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	LYS	CB-CA-C	-8.23	93.93	110.40
1	A	125	LEU	CA-CB-CG	6.33	129.85	115.30
1	A	358	LEU	CA-CB-CG	-6.16	101.13	115.30
1	A	167	LYS	N-CA-CB	5.96	121.32	110.60
1	A	351	VAL	CB-CA-C	-5.92	100.14	111.40
1	A	266	ASN	N-CA-C	5.77	126.58	111.00
1	A	225	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	225	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	555	TRP	N-CA-C	-5.61	95.86	111.00
1	A	158	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	448	ILE	CB-CA-C	-5.39	100.81	111.60
1	A	293	TRP	CA-CB-CG	5.25	123.69	113.70
1	A	259	LEU	N-CA-C	-5.21	96.93	111.00

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	5300	0	5044	249	0
2	A	214	0	0	12	0
All	All	5514	0	5044	249	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 24.

All (249) 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:167:LYS:O	1:A:167:LYS:HG2	1.42	1.14
1:A:220:THR:HB	1:A:266:ASN:HD21	1.14	1.12
1:A:220:THR:HB	1:A:266:ASN:ND2	1.65	1.10
1:A:221:LEU:H	1:A:266:ASN:CB	1.72	1.01
1:A:221:LEU:H	1:A:266:ASN:ND2	1.57	1.01
1:A:221:LEU:N	1:A:266:ASN:HD22	1.58	1.01
1:A:167:LYS:O	1:A:167:LYS:CG	2.11	0.96
1:A:282:ASN:ND2	1:A:316:ARG:HH12	1.66	0.94
1:A:376:ASP:O	1:A:377:LEU:HD12	1.68	0.93
1:A:401:ARG:H	1:A:401:ARG:HE	1.14	0.93
1:A:545:GLN:CD	1:A:549:GLY:HA2	1.92	0.90
1:A:236:VAL:HG22	1:A:250:GLU:HG3	1.54	0.90
1:A:221:LEU:N	1:A:266:ASN:HB2	1.88	0.89
1:A:598:ARG:HG3	1:A:598:ARG:HH11	1.39	0.88
1:A:431:ARG:HD3	2:A:756:HOH:O	1.75	0.85
1:A:282:ASN:HD21	1:A:316:ARG:HH12	1.22	0.84
1:A:261:ALA:O	1:A:265:GLN:HB2	1.77	0.84
1:A:221:LEU:N	1:A:266:ASN:ND2	2.20	0.83
1:A:221:LEU:H	1:A:266:ASN:CG	1.81	0.83
1:A:220:THR:CB	1:A:266:ASN:ND2	2.42	0.82
1:A:543:VAL:O	1:A:543:VAL:HG12	1.82	0.79
1:A:221:LEU:N	1:A:266:ASN:CB	2.44	0.79
1:A:265:GLN:HA	1:A:265:GLN:NE2	1.98	0.78
1:A:401:ARG:NE	1:A:401:ARG:H	1.82	0.78
1:A:34:ASP:OD2	1:A:38:LYS:HE2	1.83	0.77
1:A:584:ILE:HD12	1:A:606:THR:O	1.85	0.77
1:A:682:ARG:NH1	2:A:914:HOH:O	2.18	0.76
1:A:403:PRO:HB2	1:A:404:TYR:CD1	2.19	0.76
1:A:691:THR:HG21	1:A:695:LEU:CD2	2.16	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASP:OD1	1:A:225:ARG:HD3	1.86	0.75
1:A:434:HIS:HD2	1:A:440:ASN:ND2	1.84	0.75
1:A:460:MSE:HE2	1:A:512:ILE:HG23	1.67	0.74
1:A:479:ILE:HD12	1:A:497:GLN:HB3	1.69	0.74
1:A:655:SER:O	1:A:656:ILE:HD13	1.87	0.74
1:A:267:THR:HG22	1:A:269:SER:H	1.51	0.74
1:A:506:THR:CG2	2:A:760:HOH:O	2.37	0.73
1:A:691:THR:HG21	1:A:695:LEU:HD21	1.69	0.72
1:A:634:LYS:HG3	2:A:887:HOH:O	1.88	0.72
1:A:403:PRO:HB2	1:A:404:TYR:CE1	2.24	0.72
1:A:221:LEU:H	1:A:266:ASN:HD22	1.18	0.71
1:A:71:GLN:NE2	1:A:109:GLY:HA3	2.03	0.71
1:A:598:ARG:NH1	1:A:598:ARG:HG3	2.07	0.70
1:A:506:THR:HB	2:A:830:HOH:O	1.92	0.70
1:A:475:ASN:O	1:A:498:GLY:HA3	1.93	0.69
1:A:197:LYS:HE2	1:A:199:GLN:OE1	1.93	0.69
1:A:242:ALA:HB3	1:A:245:GLN:HB2	1.75	0.69
1:A:434:HIS:HD2	1:A:440:ASN:HD21	1.39	0.68
1:A:223:ALA:HB2	1:A:265:GLN:H	1.59	0.68
1:A:584:ILE:HD12	1:A:585:THR:H	1.59	0.68
1:A:403:PRO:HG2	1:A:404:TYR:H	1.56	0.68
1:A:318:PRO:HD3	1:A:338:VAL:HG12	1.76	0.68
1:A:455:ASP:OD2	1:A:518:ARG:HD3	1.94	0.68
1:A:506:THR:HG21	2:A:760:HOH:O	1.94	0.68
1:A:221:LEU:O	1:A:266:ASN:HB3	1.94	0.67
1:A:241:PHE:CZ	1:A:245:GLN:HB3	2.30	0.67
1:A:271:SER:OG	1:A:273:THR:HG22	1.95	0.67
1:A:264:THR:HG22	1:A:264:THR:O	1.95	0.66
1:A:215:GLY:HA3	1:A:699:ASN:ND2	2.11	0.66
1:A:267:THR:CG2	1:A:269:SER:HB3	2.27	0.65
1:A:575:SER:HB3	1:A:578:VAL:HB	1.77	0.65
1:A:221:LEU:H	1:A:266:ASN:HB2	1.42	0.65
1:A:400:ASP:HA	1:A:401:ARG:HH21	1.61	0.64
1:A:264:THR:O	1:A:264:THR:CG2	2.45	0.64
1:A:533:ARG:HG3	1:A:533:ARG:HH11	1.63	0.63
1:A:221:LEU:HB2	1:A:266:ASN:CB	2.28	0.63
1:A:663:TRP:CE2	1:A:665:VAL:HG22	2.34	0.63
1:A:203:TRP:HB2	1:A:265:GLN:HG3	1.81	0.63
1:A:375:LYS:HE2	1:A:404:TYR:CE2	2.34	0.63
1:A:375:LYS:HE2	1:A:404:TYR:HE2	1.63	0.62
1:A:245:GLN:OE1	1:A:293:TRP:CH2	2.52	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASN:O	1:A:299:ASN:ND2	2.32	0.62
1:A:637:ASN:HD21	1:A:641:GLN:HB2	1.64	0.62
1:A:215:GLY:HA3	1:A:699:ASN:HD22	1.65	0.62
1:A:220:THR:CA	1:A:266:ASN:ND2	2.64	0.61
1:A:219:THR:O	1:A:267:THR:HA	1.99	0.61
1:A:282:ASN:ND2	1:A:316:ARG:NH1	2.44	0.61
1:A:264:THR:HG23	1:A:266:ASN:ND2	2.16	0.61
1:A:517:LYS:O	1:A:518:ARG:HB3	2.01	0.61
1:A:339:ASP:H	1:A:377:LEU:HD22	1.66	0.61
1:A:265:GLN:HG2	1:A:277:TYR:CD2	2.36	0.60
1:A:548:VAL:O	1:A:548:VAL:HG12	2.03	0.59
1:A:438:VAL:HG12	1:A:438:VAL:O	2.02	0.59
1:A:264:THR:HG23	1:A:266:ASN:CG	2.23	0.59
1:A:313:ARG:HD3	1:A:339:ASP:OD2	2.03	0.58
1:A:543:VAL:O	1:A:543:VAL:CG1	2.50	0.58
1:A:167:LYS:C	1:A:169:GLU:N	2.55	0.58
1:A:266:ASN:O	1:A:267:THR:C	2.38	0.58
1:A:12:ASP:OD1	1:A:12:ASP:O	2.21	0.58
1:A:221:LEU:HB2	1:A:266:ASN:HB2	1.85	0.58
1:A:426:VAL:HG12	1:A:448:ILE:HD12	1.85	0.58
1:A:301:VAL:HG22	1:A:353:LEU:HD23	1.85	0.58
1:A:404:TYR:CD1	1:A:404:TYR:N	2.72	0.58
1:A:534:ASN:HA	1:A:558:VAL:O	2.05	0.57
1:A:265:GLN:HG2	1:A:277:TYR:HD2	1.68	0.57
1:A:43:ARG:NH2	1:A:225:ARG:NH2	2.52	0.57
1:A:101:TRP:CH2	1:A:496:LEU:HB2	2.38	0.57
1:A:241:PHE:CE2	1:A:245:GLN:HB3	2.40	0.56
1:A:191:LEU:HD12	1:A:234:ASN:O	2.06	0.56
1:A:166:HIS:HB3	1:A:168:GLU:OE1	2.06	0.56
1:A:267:THR:HG21	1:A:269:SER:HB3	1.86	0.56
1:A:101:TRP:CZ3	1:A:496:LEU:HB2	2.41	0.56
1:A:478:TYR:C	1:A:479:ILE:HD13	2.27	0.56
1:A:73:ASP:OD2	1:A:78:GLY:N	2.36	0.56
1:A:376:ASP:OD2	1:A:377:LEU:N	2.24	0.56
1:A:203:TRP:CZ3	1:A:204:ASP:HB3	2.40	0.56
1:A:406:LYS:HE3	1:A:408:GLU:OE2	2.06	0.55
1:A:98:ARG:HH22	1:A:378:SER:CB	2.19	0.55
1:A:318:PRO:HD3	1:A:338:VAL:CG1	2.37	0.55
1:A:709:TYR:HE2	1:A:711:GLU:HG2	1.72	0.55
1:A:682:ARG:C	1:A:683:LEU:HD12	2.26	0.55
1:A:672:THR:HB	1:A:719:SER:HB3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:THR:CG2	2:A:844:HOH:O	2.54	0.55
1:A:692:THR:HG22	1:A:701:ILE:HB	1.88	0.55
1:A:245:GLN:OE1	1:A:293:TRP:CZ3	2.59	0.55
1:A:28:VAL:HG13	1:A:125:LEU:HD13	1.89	0.54
1:A:506:THR:HG22	1:A:533:ARG:HB2	1.89	0.54
1:A:167:LYS:O	1:A:169:GLU:N	2.41	0.54
1:A:265:GLN:O	1:A:265:GLN:HG3	2.07	0.53
1:A:426:VAL:HG12	1:A:448:ILE:CD1	2.37	0.53
1:A:469:PRO:HB3	1:A:536:ILE:HD13	1.91	0.53
1:A:165:GLU:OE1	1:A:714:ARG:NH1	2.41	0.53
1:A:219:THR:HB	1:A:267:THR:HG23	1.90	0.53
1:A:77:MSE:HE1	1:A:532:TYR:CG	2.44	0.53
1:A:434:HIS:CD2	1:A:440:ASN:ND2	2.72	0.53
1:A:157:TRP:O	1:A:722:THR:HB	2.09	0.53
1:A:319:GLU:HG3	1:A:319:GLU:O	2.09	0.53
1:A:434:HIS:CD2	1:A:440:ASN:HD21	2.24	0.53
1:A:41:VAL:HG21	1:A:45:VAL:HA	1.91	0.52
1:A:265:GLN:HE22	1:A:273:THR:C	2.13	0.52
1:A:219:THR:CB	1:A:267:THR:HG23	2.40	0.52
1:A:447:ASN:ND2	1:A:461:GLY:HA3	2.25	0.52
1:A:592:ASN:OD1	1:A:594:THR:N	2.41	0.52
1:A:476:PRO:O	1:A:479:ILE:HD11	2.10	0.51
1:A:180:THR:OG1	1:A:189:PHE:O	2.25	0.51
1:A:236:VAL:CG2	1:A:250:GLU:HG3	2.35	0.51
1:A:584:ILE:HD12	1:A:585:THR:N	2.25	0.51
1:A:221:LEU:CB	1:A:266:ASN:HB2	2.41	0.50
1:A:168:GLU:CD	1:A:168:GLU:H	2.14	0.50
1:A:559:PRO:HD2	2:A:767:HOH:O	2.12	0.50
1:A:663:TRP:CD2	1:A:665:VAL:HG22	2.46	0.50
1:A:348:HIS:NE2	1:A:350:GLU:HG2	2.27	0.50
1:A:683:LEU:HD13	1:A:711:GLU:HG3	1.94	0.50
1:A:598:ARG:CG	1:A:598:ARG:NH1	2.72	0.49
1:A:469:PRO:HB3	1:A:536:ILE:CD1	2.43	0.49
1:A:273:THR:HG23	1:A:274:ARG:N	2.28	0.48
1:A:438:VAL:CG1	1:A:438:VAL:O	2.61	0.48
1:A:245:GLN:OE1	1:A:293:TRP:HH2	1.94	0.48
1:A:575:SER:C	1:A:577:THR:H	2.17	0.48
1:A:98:ARG:NH2	1:A:378:SER:CB	2.75	0.48
1:A:637:ASN:ND2	1:A:641:GLN:HB2	2.29	0.48
1:A:167:LYS:O	1:A:167:LYS:CD	2.61	0.48
1:A:297:TRP:HE3	1:A:301:VAL:O	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:LYS:CD	1:A:639:LYS:N	2.76	0.48
1:A:373:ARG:HG2	1:A:406:LYS:HG3	1.95	0.47
1:A:102:ARG:HH21	1:A:638:TYR:HD2	1.62	0.47
1:A:545:GLN:HA	1:A:551:ASP:HA	1.96	0.47
1:A:219:THR:OG1	1:A:267:THR:HG23	2.14	0.47
1:A:320:GLY:O	1:A:321:LEU:HG	2.13	0.47
1:A:462:ILE:HG13	1:A:510:LYS:HG2	1.97	0.47
1:A:265:GLN:OE1	1:A:274:ARG:HD2	2.15	0.46
1:A:273:THR:CG2	1:A:274:ARG:N	2.78	0.46
1:A:174:ARG:HG3	1:A:196:ASP:HB3	1.98	0.46
1:A:167:LYS:C	1:A:169:GLU:H	2.19	0.46
1:A:282:ASN:CG	1:A:316:ARG:HH12	2.18	0.46
1:A:695:LEU:HD22	1:A:695:LEU:N	2.30	0.46
1:A:478:TYR:O	1:A:479:ILE:HD13	2.16	0.46
1:A:692:THR:O	1:A:692:THR:HG23	2.16	0.46
1:A:239:TRP:CE2	1:A:241:PHE:HB3	2.50	0.46
1:A:700:TYR:CD1	1:A:700:TYR:C	2.89	0.46
1:A:340:ILE:HD12	2:A:761:HOH:O	2.16	0.45
1:A:192:TYR:O	1:A:233:ILE:HD12	2.15	0.45
1:A:448:ILE:HG22	1:A:449:SER:N	2.31	0.45
1:A:403:PRO:CB	1:A:404:TYR:CD1	2.95	0.45
1:A:611:LEU:HB3	1:A:623:THR:HG22	1.99	0.45
1:A:203:TRP:CE3	1:A:204:ASP:HB3	2.52	0.45
1:A:357:PHE:CD1	1:A:358:LEU:HD12	2.51	0.45
1:A:227:GLY:HA3	1:A:259:LEU:HB2	1.97	0.45
1:A:265:GLN:HA	1:A:273:THR:OG1	2.17	0.45
1:A:416:ASN:O	1:A:428:PRO:HD2	2.16	0.45
1:A:674:GLY:HA3	1:A:717:TYR:CZ	2.52	0.45
1:A:723:HIS:HD2	2:A:734:HOH:O	2.00	0.45
1:A:403:PRO:HG2	1:A:404:TYR:N	2.25	0.45
1:A:545:GLN:OE1	1:A:549:GLY:HA2	2.16	0.45
1:A:520:GLY:O	1:A:573:PRO:HG3	2.16	0.45
1:A:682:ARG:CZ	2:A:914:HOH:O	2.63	0.45
1:A:167:LYS:HG2	2:A:790:HOH:O	2.17	0.44
1:A:264:THR:HG23	1:A:266:ASN:OD1	2.16	0.44
1:A:267:THR:HG22	1:A:269:SER:HB3	1.97	0.44
1:A:401:ARG:N	1:A:401:ARG:HE	1.97	0.44
1:A:165:GLU:CD	1:A:714:ARG:HD2	2.38	0.44
1:A:563:VAL:HA	1:A:589:LYS:O	2.17	0.44
1:A:46:SER:HB2	1:A:72:ILE:HD11	1.99	0.44
1:A:162:ASN:HA	1:A:717:TYR:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:HG3	1:A:341:ASP:OD1	2.18	0.44
1:A:277:TYR:CD1	1:A:277:TYR:C	2.91	0.43
1:A:592:ASN:OD1	1:A:592:ASN:C	2.57	0.43
1:A:616:ARG:HB2	1:A:619:LEU:HB3	2.00	0.43
1:A:65:GLN:O	1:A:66:ARG:HB2	2.19	0.43
1:A:167:LYS:O	1:A:168:GLU:C	2.56	0.43
1:A:484:GLY:O	1:A:485:GLN:CB	2.66	0.43
1:A:575:SER:C	1:A:577:THR:N	2.71	0.43
1:A:243:PRO:O	1:A:245:GLN:HG2	2.18	0.43
1:A:363:LEU:HD21	1:A:365:LEU:HD11	2.01	0.43
1:A:574:VAL:HB	1:A:578:VAL:HG12	2.00	0.43
1:A:663:TRP:CZ2	1:A:665:VAL:HG22	2.52	0.43
1:A:26:PRO:HG2	1:A:511:GLU:OE2	2.19	0.43
1:A:583:ASN:O	1:A:607:LEU:HD12	2.19	0.43
1:A:584:ILE:CD1	1:A:606:THR:O	2.62	0.43
1:A:98:ARG:HB2	1:A:478:TYR:OH	2.19	0.43
1:A:639:LYS:HD2	1:A:639:LYS:N	2.34	0.43
1:A:666:THR:C	1:A:668:ASN:H	2.22	0.43
1:A:242:ALA:HB3	1:A:245:GLN:CB	2.46	0.42
1:A:294:ASN:HD22	1:A:304:SER:HA	1.84	0.42
1:A:357:PHE:HD1	1:A:358:LEU:HD12	1.84	0.42
1:A:66:ARG:HG3	1:A:104:GLU:HB2	2.01	0.42
1:A:564:GLU:OE2	1:A:589:LYS:HD2	2.19	0.42
1:A:34:ASP:OD2	1:A:38:LYS:CE	2.63	0.42
1:A:221:LEU:CA	1:A:266:ASN:HB2	2.48	0.42
1:A:601:ILE:HD12	1:A:633:PRO:HA	2.00	0.42
1:A:203:TRP:CH2	1:A:204:ASP:HB3	2.55	0.42
1:A:89:LYS:HA	1:A:90:PRO:HD3	1.85	0.42
1:A:95:ASN:HB2	1:A:342:LEU:CD2	2.50	0.42
1:A:265:GLN:OE1	1:A:274:ARG:CD	2.68	0.42
1:A:416:ASN:O	1:A:427:THR:HA	2.20	0.42
1:A:92:SER:HB2	1:A:310:GLU:OE2	2.19	0.41
1:A:314:ASN:OD1	1:A:316:ARG:HD2	2.20	0.41
1:A:376:ASP:C	1:A:377:LEU:HD12	2.36	0.41
1:A:533:ARG:HG3	1:A:533:ARG:NH1	2.33	0.41
1:A:163:ALA:N	1:A:716:TRP:O	2.52	0.41
1:A:344:ASP:OD1	1:A:372:GLN:NE2	2.41	0.41
1:A:402:SER:HB2	1:A:477:ASN:ND2	2.35	0.41
1:A:577:THR:HG22	1:A:613:TRP:HD1	1.86	0.41
1:A:78:GLY:HA2	1:A:79:PRO:HD3	1.80	0.41
1:A:348:HIS:CD2	1:A:348:HIS:C	2.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:PRO:CB	1:A:404:TYR:HD1	2.32	0.41
1:A:221:LEU:CA	1:A:266:ASN:CB	2.99	0.41
1:A:316:ARG:HH11	1:A:316:ARG:HB3	1.85	0.41
1:A:564:GLU:HB3	1:A:589:LYS:HD2	2.03	0.41
1:A:347:LEU:HA	1:A:347:LEU:HD13	1.77	0.41
1:A:247:LEU:HA	1:A:247:LEU:HD23	1.89	0.41
1:A:403:PRO:CG	1:A:404:TYR:HD1	2.33	0.41
1:A:221:LEU:HB2	1:A:266:ASN:HB3	2.01	0.40
1:A:577:THR:HG22	1:A:613:TRP:CD1	2.56	0.40
1:A:260:TYR:HB2	1:A:281:THR:HG23	2.04	0.40
1:A:656:ILE:HD12	1:A:677:ASN:OD1	2.22	0.40
1:A:546:ASN:N	1:A:550:THR:O	2.54	0.40
1:A:244:LEU:N	1:A:244:LEU:CD1	2.84	0.40
1:A:403:PRO:HG2	1:A:404:TYR:HD1	1.86	0.40
1:A:691:THR:HG21	1:A:695:LEU:HD22	2.02	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	672/724 (93%)	636 (95%)	29 (4%)	7 (1%)	15 23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	SER
1	A	168	GLU
1	A	548	VAL
1	A	380	ASN
1	A	403	PRO
1	A	518	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	498	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	556/587 (95%)	524 (94%)	32 (6%)	20	32

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	47	LYS
1	A	73	ASP
1	A	106	ASP
1	A	112	SER
1	A	125	LEU
1	A	247	LEU
1	A	263	ASP
1	A	264	THR
1	A	291	LEU
1	A	293	TRP
1	A	299	ASN
1	A	341	ASP
1	A	343	ASP
1	A	347	LEU
1	A	351	VAL
1	A	401	ARG
1	A	403	PRO
1	A	430	LEU
1	A	458	LEU
1	A	496	LEU
1	A	506	THR
1	A	514	LEU
1	A	563	VAL
1	A	575	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	592	ASN
1	A	597	ASP
1	A	617	GLU
1	A	624	THR
1	A	633	PRO
1	A	639	LYS
1	A	722	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	71	GLN
1	A	266	ASN
1	A	287	GLN
1	A	294	ASN
1	A	299	ASN
1	A	434	HIS
1	A	440	ASN
1	A	447	ASN
1	A	477	ASN
1	A	545	GLN
1	A	622	GLN
1	A	641	GLN
1	A	668	ASN
1	A	699	ASN
1	A	721	ASN
1	A	723	HIS

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 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 ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.