



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:20 AM UTC

PDB ID : 1F9B / pdb_00001f9b
Title : MELANIN PROTEIN INTERACTION: X-RAY STRUCTURE OF THE
COMPLEX OF MARE LACTOFERRIN WITH MELANIN MONOMERS
Authors : Kumar, S.; Singh, T.P.; Sharma, A.K.; Singh, N.; Raman, G.
Deposited on : 2000-07-10
Resolution : 2.70 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

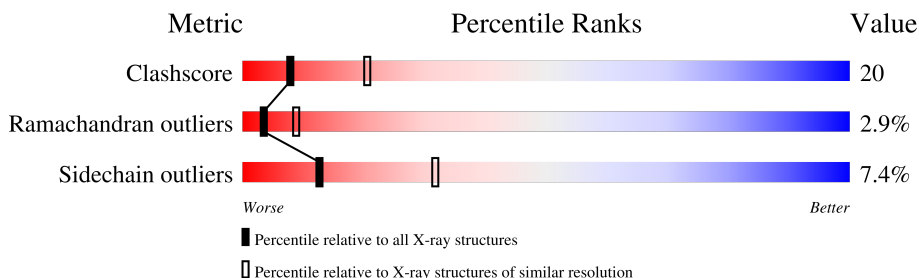
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	695	57% 36% 5% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	3ID	A	694	-	X	X	-
4	3ID	A	695	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5386 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 LACTOTRANSFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	689	Total	C	N	O	S	0	0	0
			5281	3299	937	1008	37			

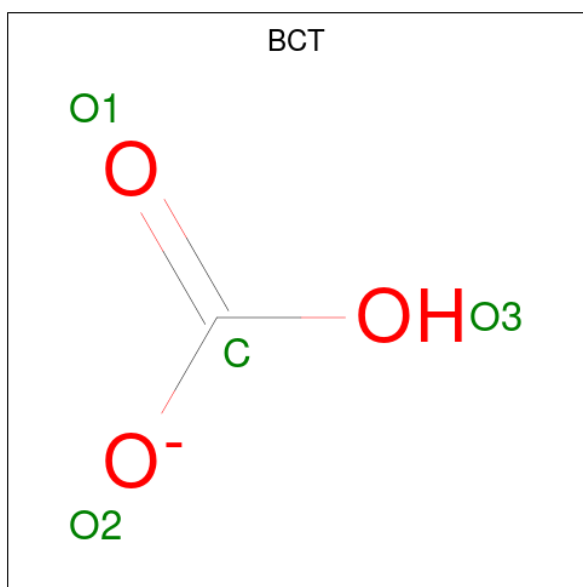
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	GLU	ASP	SEE REMARK 999	UNP O77811
A	269	LYS	ARG	SEE REMARK 999	UNP O77811
A	295	GLU	ASN	SEE REMARK 999	UNP O77811
A	296	GLN	LYS	SEE REMARK 999	UNP O77811

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

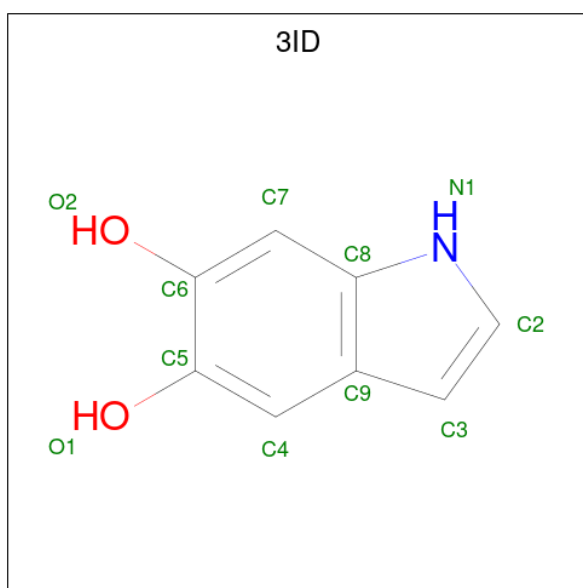
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		

- Molecule 3 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is 3H-INDOLE-5,6-DIOL (CCD ID: 3ID) (formula: C₈H₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			11	8	1	2		
4	A	1	Total	C	N	O	0	0
			11	8	1	2		

- Molecule 5 is water.

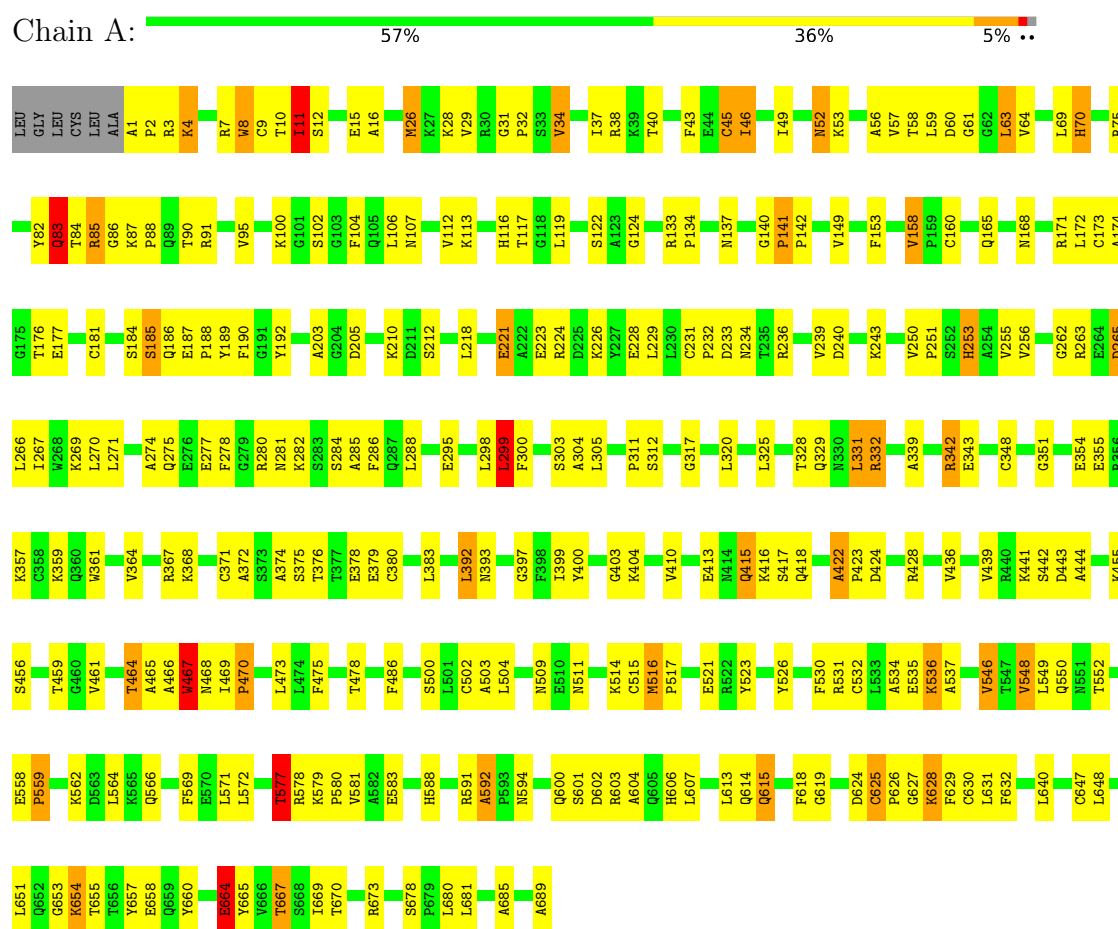
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	73	Total 73	O 73	0	0

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. 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: LACTOTRANSFERRIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.04Å 99.81Å 103.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	91.0 (15.00-2.70)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.215 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5386	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3ID, BCT, FE

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	0.81	1/5392 (0.0%)	1.27	57/7298 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	TRP	NE1-CE2	-5.43	1.31	1.37

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	VAL	N-CA-C	-13.11	97.58	110.30
1	A	368	LYS	N-CA-C	-11.13	99.09	112.89
1	A	399	ILE	N-CA-C	-10.02	100.40	110.62
1	A	158	VAL	N-CA-C	-9.55	98.69	108.15
1	A	312	SER	N-CA-C	9.50	122.84	111.82
1	A	141	PRO	N-CA-C	8.54	121.12	110.70
1	A	70	HIS	N-CA-C	7.64	126.69	109.81
1	A	628	LYS	N-CA-C	7.61	123.71	113.97
1	A	468	ASN	N-CA-C	7.60	120.23	111.11
1	A	46	ILE	N-CA-C	-7.59	103.13	110.42
1	A	548	VAL	N-CA-C	-7.35	103.62	110.53
1	A	284	SER	N-CA-C	-7.29	105.56	114.75
1	A	606	HIS	N-CA-C	-7.14	103.43	111.14
1	A	592	ALA	N-CA-C	7.12	119.73	110.40
1	A	367	ARG	N-CA-C	6.95	121.14	112.24
1	A	282	LYS	N-CA-C	-6.94	103.79	111.36
1	A	509	ASN	N-CA-C	6.94	118.85	111.28
1	A	503	ALA	N-CA-C	6.90	118.45	111.07
1	A	299	LEU	O-C-N	-6.86	113.46	122.59
1	A	140	GLY	CA-C-N	6.61	127.19	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLY	C-N-CA	6.61	127.19	120.38
1	A	31	GLY	CA-C-N	6.54	126.93	119.93
1	A	31	GLY	C-N-CA	6.54	126.93	119.93
1	A	467	TRP	N-CA-C	6.30	124.21	110.80
1	A	253	HIS	N-CA-C	-6.29	102.67	110.41
1	A	526	TYR	CB-CA-C	-6.22	99.13	110.63
1	A	577	THR	N-CA-C	6.21	117.89	110.19
1	A	456	SER	N-CA-C	6.14	119.20	109.50
1	A	536	LYS	N-CA-C	6.12	119.98	111.90
1	A	558	GLU	CA-C-N	6.11	127.48	119.84
1	A	558	GLU	C-N-CA	6.11	127.48	119.84
1	A	82	TYR	N-CA-C	6.09	117.83	109.18
1	A	137	ASN	N-CA-C	-6.06	103.45	111.02
1	A	331	LEU	N-CA-C	-5.96	105.66	113.17
1	A	11	ILE	N-CA-C	5.90	119.86	113.43
1	A	104	PHE	N-CA-C	5.87	117.90	110.33
1	A	304	ALA	N-CA-C	-5.85	101.01	110.32
1	A	511	ASN	N-CA-C	5.79	119.66	112.24
1	A	226	LYS	N-CA-C	-5.76	106.23	113.20
1	A	601	SER	CA-C-N	5.75	128.24	120.65
1	A	601	SER	C-N-CA	5.75	128.24	120.65
1	A	372	ALA	N-CA-C	-5.74	100.33	109.23
1	A	600	GLN	N-CA-C	-5.73	102.96	110.53
1	A	660	TYR	N-CA-C	5.66	117.25	111.14
1	A	371	CYS	N-CA-C	5.59	118.68	109.85
1	A	102	SER	N-CA-C	-5.57	106.53	113.38
1	A	569	PHE	N-CA-C	5.52	118.47	109.59
1	A	275	GLN	CB-CA-C	-5.44	101.59	110.85
1	A	171	ARG	N-CA-C	5.32	117.76	111.33
1	A	190	PHE	N-CA-C	5.26	118.13	109.76
1	A	351	GLY	CA-C-N	5.24	126.39	119.84
1	A	351	GLY	C-N-CA	5.24	126.39	119.84
1	A	45	CYS	N-CA-C	-5.19	105.80	111.82
1	A	85	ARG	N-CA-C	-5.06	103.17	113.29
1	A	464	THR	N-CA-C	5.06	121.58	110.80
1	A	549	LEU	N-CA-C	5.03	117.41	111.33
1	A	418	GLN	N-CA-C	5.01	116.94	108.02

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	5281	0	5139	207	0
2	A	2	0	0	0	0
3	A	8	0	0	1	0
4	A	22	0	14	22	0
5	A	73	0	0	5	0
All	All	5386	0	5153	207	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 20.

All (207) 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:8:TRP:HE1	4:A:694:3ID:C5	1.59	1.14
1:A:57:VAL:HA	4:A:694:3ID:H4	1.40	1.01
1:A:15:GLU:CD	4:A:694:3ID:HN1	1.71	0.99
1:A:10:THR:HA	4:A:694:3ID:H2	1.62	0.82
1:A:29:VAL:HG11	1:A:277:GLU:HG2	1.60	0.81
1:A:106:LEU:HD23	1:A:232:PRO:HA	1.60	0.81
1:A:8:TRP:NE1	4:A:694:3ID:C5	2.42	0.79
1:A:422:ALA:HB1	1:A:423:PRO:HD2	1.66	0.78
1:A:251:PRO:HB3	5:A:701:HOH:O	1.83	0.77
1:A:329:GLN:HA	1:A:332:ARG:HD3	1.68	0.75
1:A:1:ALA:HB3	1:A:2:PRO:HD3	1.68	0.75
1:A:504:LEU:HD13	1:A:537:ALA:O	1.88	0.74
1:A:12:SER:HB3	1:A:184:SER:HB2	1.70	0.74
1:A:57:VAL:HA	4:A:694:3ID:C4	2.17	0.74
1:A:87:LYS:H	1:A:87:LYS:HD2	1.52	0.73
1:A:16:ALA:HB2	1:A:38:ARG:HD2	1.68	0.73
1:A:376:THR:HG22	1:A:517:PRO:HG2	1.70	0.73
1:A:466:ALA:O	1:A:470:PRO:HD2	1.87	0.73
1:A:8:TRP:HE1	4:A:694:3ID:C4	2.02	0.73
1:A:625:CYS:HB3	1:A:626:PRO:HD3	1.71	0.72
1:A:141:PRO:HG2	1:A:142:PRO:HD3	1.72	0.71
1:A:376:THR:HG22	1:A:517:PRO:CG	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:THR:O	1:A:85:ARG:HB3	1.92	0.70
1:A:49:ILE:CD1	1:A:57:VAL:HG22	2.22	0.69
1:A:7:ARG:HH22	1:A:52:ASN:ND2	1.91	0.68
1:A:502:CYS:O	1:A:514:LYS:HE2	1.93	0.68
1:A:174:ALA:O	1:A:188:PRO:HD2	1.94	0.68
1:A:665:TYR:CZ	1:A:669:ILE:HD11	2.30	0.67
1:A:8:TRP:NE1	4:A:694:3ID:C4	2.58	0.66
1:A:185:SER:HB2	1:A:295:GLU:HG2	1.78	0.66
1:A:580:PRO:HD2	1:A:583:GLU:HG3	1.77	0.66
1:A:106:LEU:CD2	1:A:232:PRO:HA	2.25	0.66
1:A:210:LYS:HD3	1:A:212:SER:OG	1.96	0.65
1:A:571:LEU:HD21	1:A:581:VAL:HG13	1.79	0.65
1:A:348:CYS:SG	1:A:383:LEU:HD12	2.37	0.65
1:A:3:ARG:HG2	1:A:266:LEU:HD11	1.77	0.65
1:A:117:THR:OG1	1:A:124:GLY:HA3	1.96	0.64
1:A:149:VAL:HG13	1:A:153:PHE:HD2	1.62	0.64
1:A:10:THR:HA	4:A:694:3ID:C2	2.28	0.63
1:A:354:GLU:CD	4:A:695:3ID:HN1	2.06	0.63
1:A:357:LYS:HG2	1:A:640:LEU:HD12	1.81	0.63
1:A:45:CYS:HB3	1:A:57:VAL:HG11	1.81	0.62
1:A:57:VAL:HG12	4:A:694:3ID:C3	2.30	0.62
1:A:577:THR:HG22	1:A:578:ARG:H	1.66	0.61
1:A:328:THR:HG22	1:A:332:ARG:NH1	2.16	0.61
1:A:243:LYS:HE2	5:A:732:HOH:O	2.01	0.61
1:A:56:ALA:O	1:A:57:VAL:HG13	2.01	0.60
1:A:116:HIS:CG	1:A:158:VAL:HG22	2.35	0.60
1:A:119:LEU:HB3	1:A:160:CYS:HB2	1.83	0.60
1:A:149:VAL:HG13	1:A:153:PHE:CD2	2.37	0.60
1:A:653:GLY:O	1:A:655:THR:HG23	2.02	0.60
1:A:11:ILE:HG23	4:A:694:3ID:C2	2.32	0.59
1:A:632:PHE:HE2	1:A:647:CYS:HA	1.68	0.59
1:A:10:THR:CA	4:A:694:3ID:H2	2.33	0.59
1:A:122:SER:HB3	1:A:250:VAL:HG11	1.85	0.59
1:A:478:THR:HG21	1:A:486:PHE:CE2	2.38	0.59
1:A:521:GLU:OE2	1:A:523:TYR:HB2	2.03	0.59
1:A:49:ILE:HD11	1:A:57:VAL:HG22	1.84	0.58
1:A:579:LYS:HB3	1:A:583:GLU:HG3	1.85	0.58
1:A:49:ILE:HD12	1:A:57:VAL:HG22	1.85	0.58
1:A:615:GLN:HE22	1:A:648:LEU:H	1.52	0.58
1:A:516:MET:HG3	1:A:517:PRO:HD2	1.87	0.57
1:A:469:ILE:O	1:A:473:LEU:HG	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:TYR:O	1:A:669:ILE:HG13	2.05	0.57
1:A:37:ILE:HD12	1:A:53:LYS:HZ3	1.70	0.57
1:A:632:PHE:CE2	1:A:647:CYS:HA	2.40	0.57
1:A:3:ARG:CG	1:A:266:LEU:HD11	2.35	0.56
1:A:88:PRO:HB3	1:A:305:LEU:HD12	1.86	0.56
1:A:265:ASP:O	1:A:269:LYS:HG3	2.05	0.56
1:A:251:PRO:HG3	1:A:320:LEU:HD23	1.88	0.56
1:A:34:VAL:HG13	1:A:270:LEU:HD21	1.87	0.55
1:A:342:ARG:HG3	1:A:342:ARG:HH11	1.71	0.55
1:A:299:LEU:HA	4:A:694:3ID:C7	2.36	0.55
1:A:415:GLN:O	1:A:417:SER:N	2.40	0.55
1:A:552:THR:OG1	1:A:566:GLN:HG2	2.06	0.55
1:A:442:SER:O	1:A:444:ALA:N	2.39	0.54
1:A:422:ALA:HB1	1:A:423:PRO:CD	2.37	0.54
1:A:546:VAL:HG13	1:A:550:GLN:HE21	1.73	0.54
1:A:58:THR:H	4:A:694:3ID:C5	2.21	0.53
1:A:274:ALA:HB1	1:A:288:LEU:HD22	1.89	0.53
1:A:133:ARG:HB3	1:A:134:PRO:HD3	1.90	0.53
1:A:376:THR:HB	5:A:758:HOH:O	2.08	0.53
1:A:603:ARG:O	1:A:607:LEU:HB2	2.09	0.53
1:A:83:GLN:CG	1:A:84:THR:H	2.21	0.53
1:A:85:ARG:NH1	1:A:243:LYS:HZ2	2.06	0.53
1:A:298:LEU:O	1:A:300:PHE:N	2.42	0.53
1:A:625:CYS:C	1:A:630:CYS:SG	2.92	0.53
1:A:329:GLN:O	1:A:332:ARG:HG2	2.10	0.52
1:A:83:GLN:HE21	1:A:85:ARG:N	2.08	0.52
1:A:228:GLU:OE1	1:A:236:ARG:HD3	2.09	0.52
1:A:173:CYS:HB3	1:A:187:GLU:OE1	2.08	0.52
1:A:629:PHE:HE2	1:A:631:LEU:HD13	1.74	0.52
1:A:651:LEU:O	1:A:654:LYS:HG2	2.09	0.52
1:A:439:VAL:HG11	1:A:572:LEU:HD11	1.91	0.51
1:A:364:VAL:HG13	1:A:628:LYS:HE2	1.92	0.51
1:A:465:ALA:HB3	3:A:693:BCT:O3	2.10	0.51
1:A:534:ALA:C	1:A:536:LYS:H	2.18	0.51
1:A:113:LYS:HB3	1:A:172:LEU:HD11	1.92	0.51
1:A:339:ALA:O	1:A:343:GLU:HG3	2.08	0.51
1:A:546:VAL:CG1	1:A:550:GLN:HE21	2.23	0.51
1:A:615:GLN:HE22	1:A:648:LEU:N	2.09	0.50
1:A:298:LEU:O	1:A:299:LEU:C	2.52	0.50
1:A:530:PHE:CZ	1:A:548:VAL:HG13	2.46	0.50
1:A:29:VAL:HG12	1:A:29:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:O	1:A:53:LYS:HD3	2.11	0.50
1:A:184:SER:C	1:A:186:GLN:H	2.20	0.50
1:A:393:ASN:ND2	1:A:413:GLU:OE2	2.45	0.50
1:A:685:ALA:O	1:A:689:ALA:HB2	2.12	0.50
1:A:112:VAL:HG13	1:A:205:ASP:HB2	1.93	0.49
1:A:464:THR:HG21	1:A:592:ALA:HB1	1.94	0.49
1:A:221:GLU:HA	1:A:224:ARG:NH1	2.27	0.49
1:A:424:ASP:O	1:A:428:ARG:N	2.46	0.49
1:A:459:THR:HG23	1:A:466:ALA:HB2	1.95	0.49
1:A:342:ARG:HG3	1:A:342:ARG:NH1	2.27	0.49
1:A:172:LEU:HD13	1:A:203:ALA:O	2.12	0.49
1:A:15:GLU:HG2	1:A:299:LEU:HD23	1.94	0.49
1:A:133:ARG:N	1:A:134:PRO:CD	2.76	0.49
1:A:355:GLU:O	1:A:359:LYS:HG2	2.13	0.49
1:A:112:VAL:CG1	1:A:205:ASP:HB2	2.42	0.48
1:A:59:LEU:O	1:A:253:HIS:HB3	2.12	0.48
1:A:43:PHE:O	1:A:46:ILE:HB	2.13	0.48
1:A:625:CYS:O	1:A:626:PRO:C	2.55	0.48
1:A:422:ALA:CB	1:A:423:PRO:HD2	2.41	0.48
1:A:45:CYS:CB	1:A:57:VAL:HG11	2.44	0.47
1:A:95:VAL:HB	1:A:229:LEU:HD22	1.95	0.47
1:A:8:TRP:HZ2	4:A:694:3ID:H1O	1.61	0.47
1:A:9:CYS:HB3	1:A:57:VAL:CG1	2.44	0.47
1:A:436:VAL:HG12	1:A:588:HIS:HA	1.96	0.47
1:A:251:PRO:HG3	1:A:320:LEU:CD2	2.44	0.47
1:A:85:ARG:HG2	1:A:85:ARG:O	2.13	0.47
1:A:475:PHE:O	1:A:475:PHE:CD1	2.68	0.47
1:A:624:ASP:HB3	1:A:628:LYS:HG2	1.95	0.47
1:A:83:GLN:HG3	1:A:84:THR:H	1.80	0.47
1:A:218:LEU:HB3	1:A:223:GLU:HB2	1.97	0.47
1:A:523:TYR:CE2	1:A:532:CYS:HA	2.50	0.46
1:A:580:PRO:HD2	1:A:583:GLU:CG	2.42	0.46
1:A:615:GLN:O	1:A:619:GLY:HA3	2.15	0.46
1:A:84:THR:C	1:A:86:GLY:H	2.21	0.46
1:A:87:LYS:HD2	1:A:87:LYS:N	2.27	0.46
1:A:299:LEU:C	4:A:694:3ID:O2	2.59	0.46
1:A:63:LEU:HD23	1:A:63:LEU:N	2.30	0.46
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.74	0.46
1:A:187:GLU:OE2	1:A:189:TYR:HB2	2.16	0.46
1:A:397:GLY:O	1:A:400:TYR:HB3	2.16	0.46
1:A:552:THR:HG22	1:A:564:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:GLN:HE21	1:A:615:GLN:HB2	1.55	0.46
1:A:60:ASP:O	1:A:61:GLY:C	2.58	0.45
1:A:58:THR:N	4:A:694:3ID:O1	2.50	0.45
1:A:57:VAL:HG23	1:A:256:VAL:HG22	1.98	0.45
1:A:60:ASP:HA	1:A:253:HIS:CD2	2.51	0.45
1:A:461:VAL:HG12	1:A:467:TRP:CE3	2.51	0.45
1:A:231:CYS:HB2	1:A:233:ASP:OD1	2.17	0.45
1:A:317:GLY:HA2	1:A:325:LEU:HD11	1.97	0.45
1:A:331:LEU:HD23	5:A:745:HOH:O	2.15	0.45
1:A:26:MET:HG3	1:A:32:PRO:O	2.16	0.45
1:A:439:VAL:CG1	1:A:572:LEU:HD11	2.47	0.45
1:A:85:ARG:NH1	1:A:243:LYS:NZ	2.65	0.44
1:A:262:GLY:O	1:A:263:ARG:HB2	2.17	0.44
1:A:84:THR:C	1:A:86:GLY:N	2.76	0.44
1:A:361:TRP:HB2	1:A:629:PHE:CZ	2.52	0.44
1:A:57:VAL:O	1:A:256:VAL:HG22	2.16	0.44
1:A:59:LEU:HD12	1:A:256:VAL:HG11	1.99	0.44
1:A:410:VAL:HG11	1:A:607:LEU:HD12	1.99	0.44
1:A:466:ALA:O	1:A:467:TRP:C	2.60	0.44
1:A:523:TYR:CZ	1:A:532:CYS:HA	2.53	0.44
1:A:8:TRP:CH2	1:A:271:LEU:HD21	2.53	0.43
1:A:328:THR:O	1:A:332:ARG:HD2	2.19	0.43
1:A:192:TYR:CE1	1:A:210:LYS:HB2	2.53	0.43
1:A:28:LYS:NZ	1:A:285:ALA:HB1	2.32	0.43
1:A:107:ASN:N	1:A:234:ASN:OD1	2.51	0.43
1:A:329:GLN:HA	1:A:332:ARG:CD	2.43	0.43
1:A:278:PHE:CG	1:A:286:PHE:HD2	2.36	0.43
1:A:657:TYR:CE1	1:A:658:GLU:HG3	2.52	0.43
1:A:678:SER:OG	1:A:681:LEU:HB2	2.18	0.43
1:A:100:LYS:HG2	1:A:228:GLU:HG3	2.01	0.43
1:A:9:CYS:O	4:A:694:3ID:C2	2.67	0.43
1:A:664:GLU:N	1:A:664:GLU:CD	2.75	0.43
1:A:669:ILE:O	1:A:673:ARG:HG3	2.19	0.43
1:A:34:VAL:HG13	1:A:270:LEU:CD2	2.49	0.43
1:A:403:GLY:HA3	1:A:657:TYR:CD2	2.53	0.43
1:A:250:VAL:HB	1:A:251:PRO:HD2	2.01	0.42
1:A:116:HIS:CD2	1:A:158:VAL:HG22	2.54	0.42
1:A:546:VAL:CG1	1:A:550:GLN:NE2	2.82	0.42
1:A:45:CYS:O	1:A:49:ILE:N	2.46	0.42
1:A:267:ILE:O	1:A:270:LEU:HB3	2.20	0.42
1:A:280:ARG:NH2	1:A:303:SER:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:HG22	1:A:517:PRO:HG3	1.99	0.42
1:A:455:LYS:HB3	1:A:504:LEU:HD11	2.02	0.42
1:A:613:LEU:O	1:A:614:GLN:C	2.62	0.42
1:A:251:PRO:O	1:A:251:PRO:HG2	2.20	0.41
1:A:422:ALA:C	1:A:424:ASP:H	2.28	0.41
1:A:374:ALA:HB1	1:A:379:GLU:CB	2.50	0.41
1:A:531:ARG:O	1:A:532:CYS:C	2.64	0.41
1:A:234:ASN:HA	5:A:736:HOH:O	2.20	0.41
1:A:415:GLN:HE22	1:A:594:ASN:HD21	1.68	0.41
1:A:380:CYS:HB3	1:A:392:LEU:HD21	2.02	0.41
1:A:629:PHE:HE2	1:A:631:LEU:CD1	2.33	0.41
1:A:149:VAL:CG1	1:A:153:PHE:HD2	2.33	0.41
1:A:478:THR:HG21	1:A:486:PHE:CD2	2.55	0.41
1:A:15:GLU:OE1	4:A:694:3ID:N1	2.51	0.41
1:A:57:VAL:HG12	4:A:694:3ID:H3	2.03	0.41
1:A:410:VAL:HG22	1:A:604:ALA:HB1	2.02	0.41
1:A:625:CYS:HA	1:A:629:PHE:O	2.19	0.41
1:A:15:GLU:CD	4:A:694:3ID:N1	2.56	0.41
1:A:173:CYS:HB3	1:A:187:GLU:CD	2.46	0.40
1:A:664:GLU:O	1:A:667:THR:N	2.54	0.40
1:A:439:VAL:HG21	1:A:572:LEU:HD21	2.04	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	687/695 (99%)	600 (87%)	67 (10%)	20 (3%)	3 9

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ASN
1	A	467	TRP
1	A	562	LYS
1	A	4	LYS
1	A	416	LYS
1	A	422	ALA
1	A	627	GLY
1	A	654	LYS
1	A	70	HIS
1	A	83	GLN
1	A	176	THR
1	A	177	GLU
1	A	221	GLU
1	A	443	ASP
1	A	559	PRO
1	A	664	GLU
1	A	535	GLU
1	A	299	LEU
1	A	625	CYS
1	A	470	PRO

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	565/571 (99%)	523 (93%)	42 (7%)	13	32

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	11	ILE
1	A	26	MET
1	A	34	VAL
1	A	40	THR
1	A	52	ASN
1	A	63	LEU

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Mol	Chain	Res	Type
1	A	75	ARG
1	A	83	GLN
1	A	90	THR
1	A	91	ARG
1	A	165	GLN
1	A	168	ASN
1	A	181	CYS
1	A	185	SER
1	A	239	VAL
1	A	240	ASP
1	A	255	VAL
1	A	265	ASP
1	A	311	PRO
1	A	332	ARG
1	A	342	ARG
1	A	375	SER
1	A	378	GLU
1	A	392	LEU
1	A	404	LYS
1	A	415	GLN
1	A	441	LYS
1	A	500	SER
1	A	515	CYS
1	A	516	MET
1	A	546	VAL
1	A	559	PRO
1	A	577	THR
1	A	591	ARG
1	A	602	ASP
1	A	615	GLN
1	A	618	PHE
1	A	664	GLU
1	A	667	THR
1	A	670	THR
1	A	680	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	23	GLN
1	A	25	ASN
1	A	52	ASN

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Mol	Chain	Res	Type
1	A	83	GLN
1	A	137	ASN
1	A	168	ASN
1	A	186	GLN
1	A	201	ASN
1	A	330	ASN
1	A	415	GLN
1	A	421	ASN
1	A	513	ASN
1	A	550	GLN
1	A	556	ASN
1	A	606	HIS
1	A	615	GLN
1	A	621	ASN
1	A	642	ASN
1	A	659	GLN

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	BCT	A	692	2	3,3,3	0.30	0	2,3,3	2.67	1 (50%)
4	3ID	A	695	-	12,12,12	5.33	9 (75%)	16,17,17	5.70	6 (37%)
3	BCT	A	693	2	3,3,3	0.49	0	2,3,3	0.62	0
4	3ID	A	694	-	12,12,12	3.41	8 (66%)	16,17,17	5.36	8 (50%)

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
4	3ID	A	695	-	-	-	0/2/2/2
4	3ID	A	694	-	-	-	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	695	3ID	C2-C3	11.96	1.58	1.36
4	A	694	3ID	C2-C3	7.09	1.49	1.36
4	A	695	3ID	C6-C5	6.64	1.51	1.40
4	A	695	3ID	C9-C3	6.02	1.61	1.43
4	A	695	3ID	O1-C5	5.49	1.47	1.36
4	A	695	3ID	C4-C5	5.43	1.46	1.38
4	A	695	3ID	C7-C6	4.96	1.46	1.38
4	A	694	3ID	C6-C5	-4.85	1.31	1.40
4	A	694	3ID	O1-C5	4.44	1.45	1.36
4	A	695	3ID	O2-C6	4.19	1.44	1.36
4	A	694	3ID	O2-C6	3.53	1.43	1.36
4	A	694	3ID	C7-C6	3.19	1.43	1.38
4	A	694	3ID	C8-N1	2.60	1.42	1.37
4	A	695	3ID	C7-C8	2.27	1.43	1.39
4	A	694	3ID	C4-C9	-2.26	1.37	1.40
4	A	694	3ID	C4-C5	2.25	1.42	1.38
4	A	695	3ID	C2-N1	2.16	1.42	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	695	3ID	C3-C2-N1	-17.19	90.40	110.25
4	A	694	3ID	C9-C3-C2	-14.40	89.49	107.05
4	A	695	3ID	C8-C9-C3	-12.95	98.40	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	694	3ID	C8-N1-C2	-10.98	100.89	108.91
4	A	694	3ID	C7-C8-C9	-6.16	116.48	122.59
4	A	694	3ID	C8-C9-C3	-5.95	102.83	106.59
4	A	695	3ID	C9-C8-N1	-5.49	103.13	107.53
4	A	694	3ID	C7-C6-C5	-4.74	115.50	119.89
3	A	692	BCT	O2-C-O1	-3.72	110.17	119.68
4	A	694	3ID	C4-C9-C8	-2.97	117.29	119.13
4	A	694	3ID	O2-C6-C7	2.85	127.15	119.45
4	A	694	3ID	C7-C8-N1	2.42	135.36	131.62
4	A	695	3ID	C4-C5-C6	-2.19	117.86	119.89
4	A	695	3ID	C8-N1-C2	2.06	110.42	108.91
4	A	695	3ID	C7-C8-N1	-2.03	128.50	131.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	695	3ID	1	0
3	A	693	BCT	1	0
4	A	694	3ID	21	0

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

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.