



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:21 PM GMT

PDB ID : 1F9B  
Title : MELANIN PROTEIN INTERACTION: X-RAY STRUCTURE OF THE  
COMPLEX OF MARE LACTOFERRIN WITH MELANIN MONOMERS  
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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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

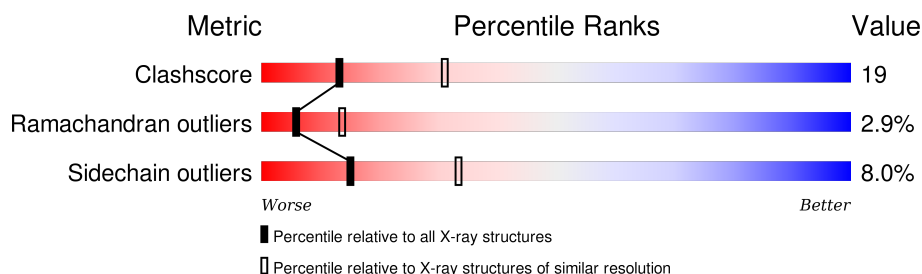
# 1 Overall quality at a glance

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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	695	 62% 32% . .

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	-

## 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			

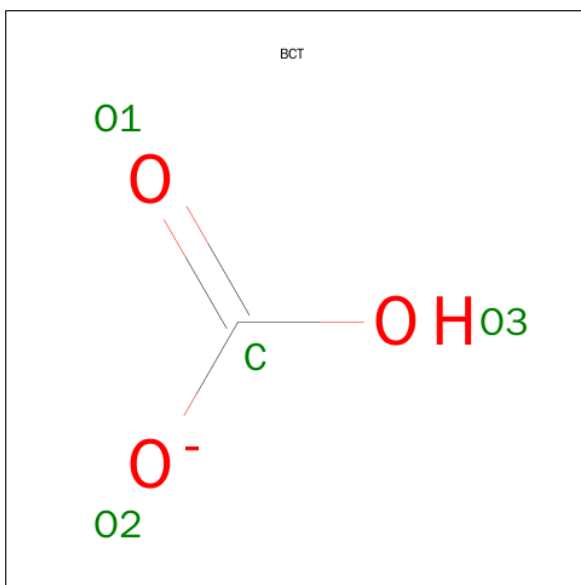
There are 4 discrepancies between the modelled and reference sequences:

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 (three-letter code: FE) (formula: Fe).

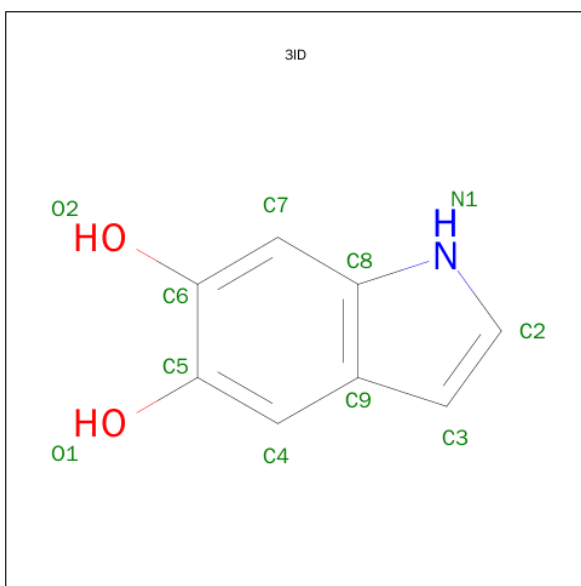
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		

- Molecule 3 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



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 (three-letter code: 3ID) (formula:  $C_8H_7NO_2$ ).



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.

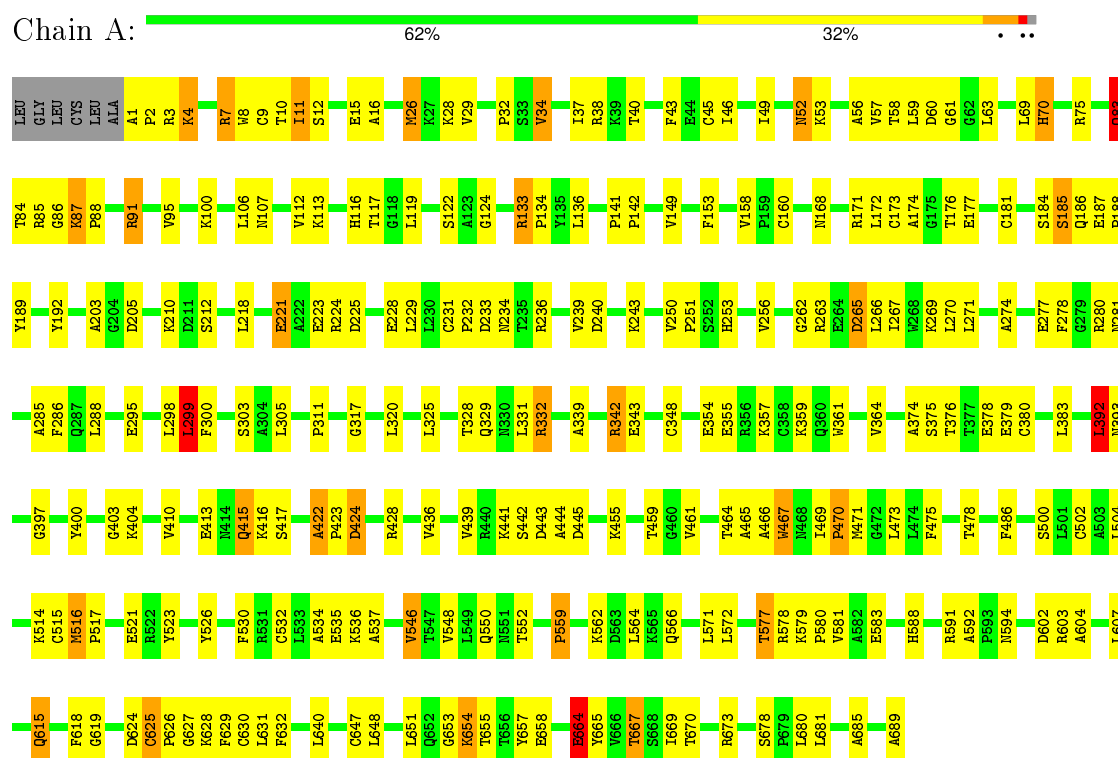
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	73	Total	O	0	0
			73	73		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

Note EDS was not executed.

#### • Molecule 1: LACTOTRANSFERRIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	30.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.63	0/5392	0.90	8/7298 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	392	LEU	CA-CB-CG	7.21	131.87	115.30
1	A	526	TYR	CB-CG-CD2	-6.56	117.07	121.00
1	A	7	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	91	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	A	70	HIS	N-CA-C	5.81	126.69	111.00
1	A	299	LEU	O-C-N	-5.77	113.46	122.70
1	A	526	TYR	CB-CA-C	-5.63	99.13	110.40
1	A	136	LEU	CB-CG-CD1	-5.01	102.48	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	5281	0	5139	198	0
2	A	2	0	0	0	0
3	A	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	22	0	14	21	0
5	A	73	0	0	5	0
All	All	5386	0	5153	198	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 19.

All (198) 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	0.94
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:149:VAL:HG13	1:A:153:PHE:CD2	2.37	0.60
1:A:119:LEU:HB3	1:A:160:CYS:HB2	1.83	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:354:GLU:CD	4:A:695:3ID:HN1	2.06	0.58
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:37:ILE:HD12	1:A:53:LYS:HZ3	1.69	0.57
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
1:A:665:TYR:O	1:A:669:ILE:HG13	2.05	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:HH11	1:A:342:ARG:HG3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:298:LEU:O	1:A:300:PHE:N	2.42	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:465:ALA:HB3	3:A:693:BCT:O3	2.10	0.51
1:A:364:VAL:HG13	1:A:628:LYS:HE2	1.92	0.51
1:A:339:ALA:O	1:A:343:GLU:HG3	2.08	0.51
1:A:113:LYS:HB3	1:A:172:LEU:HD11	1.92	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: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
1:A:53:LYS:O	1:A:53:LYS:HD3	2.11	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:459:THR:HG23	1:A:466:ALA:HB2	1.95	0.49
1:A:424:ASP:O	1:A:428:ARG:N	2.46	0.49
1:A:342:ARG:NH1	1:A:342:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C	1:A:630:CYS:SG	2.92	0.48
1:A:85:ARG:O	1:A:85:ARG:HG2	2.13	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:624:ASP:HB3	1:A:628:LYS:HG2	1.95	0.47
1:A:475:PHE:CD1	1:A:475:PHE:O	2.68	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:580:PRO:HD2	1:A:583:GLU:CG	2.42	0.46
1:A:523:TYR:CE2	1:A:532:CYS:HA	2.50	0.46
1:A:615:GLN:O	1:A:619:GLY:HA3	2.15	0.46
1:A:534:ALA:C	1:A:536:LYS:H	2.18	0.46
1:A:87:LYS:N	1:A:87:LYS:HD2	2.27	0.46
1:A:63:LEU:N	1:A:63:LEU:HD23	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:615:GLN:HE21	1:A:615:GLN:HB2	1.55	0.46
1:A:552:THR:HG22	1:A:564:LEU:HB3	1.98	0.46
1:A:298:LEU:O	1:A:299:LEU:C	2.52	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:184:SER:C	1:A:186:GLN:H	2.20	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:85:ARG:NH1	1:A:243:LYS:NZ	2.65	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:262:GLY:O	1:A:263:ARG:HB2	2.17	0.44
1:A:361:TRP:HB2	1:A:629:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:625:CYS:O	1:A:626:PRO:C	2.55	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: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:455:LYS:HB3	1:A:504:LEU:HD11	2.02	0.42
1:A:376:THR:HG22	1:A:517:PRO:HG3	1.99	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
1:A:251:PRO:HG2	1:A:251:PRO:O	2.20	0.41
1:A:299:LEU:C	4:A:694:3ID:O2	2.59	0.41
1:A:84:THR:C	1:A:86:GLY:H	2.21	0.41
1:A:374:ALA:HB1	1:A:379:GLU:CB	2.50	0.41
1:A:60:ASP:O	1:A:61:GLY:C	2.58	0.41
1:A:415:GLN:HE22	1:A:594:ASN:HD21	1.68	0.41
1:A:234:ASN:HA	5:A:736:HOH:O	2.20	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:57:VAL:HG12	4:A:694:3ID:H3	2.03	0.41
1:A:15:GLU:OE1	4:A:694:3ID:N1	2.51	0.41
1:A:625:CYS:HA	1:A:629:PHE:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:VAL:HG22	1:A:604:ALA:HB1	2.02	0.41
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%)	6	14

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

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Mol	Chain	Res	Type
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%)	520 (92%)	45 (8%)	15	33

All (45) 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	75	ARG
1	A	83	GLN
1	A	87	LYS
1	A	91	ARG
1	A	133	ARG
1	A	168	ASN
1	A	171	ARG
1	A	181	CYS
1	A	185	SER
1	A	225	ASP
1	A	239	VAL
1	A	240	ASP
1	A	265	ASP
1	A	311	PRO
1	A	332	ARG
1	A	342	ARG
1	A	375	SER
1	A	378	GLU

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Mol	Chain	Res	Type
1	A	392	LEU
1	A	404	LYS
1	A	415	GLN
1	A	424	ASP
1	A	441	LYS
1	A	445	ASP
1	A	471	MET
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	25	ASN
1	A	52	ASN
1	A	83	GLN
1	A	137	ASN
1	A	201	ASN
1	A	330	ASN
1	A	415	GLN
1	A	550	GLN
1	A	556	ASN
1	A	615	GLN
1	A	621	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	0,3,3	0.00	-	0,3,3	0.00	-
3	BCT	A	693	2	0,3,3	0.00	-	0,3,3	0.00	-
4	3ID	A	694	-	10,12,12	3.40	6 (60%)	14,17,17	3.33	7 (50%)
4	3ID	A	695	-	10,12,12	4.91	6 (60%)	14,17,17	2.99	5 (35%)

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	BCT	A	692	2	-	0/0/0/0	0/0/0/0
3	BCT	A	693	2	-	0/0/0/0	0/0/0/0
4	3ID	A	694	-	-	0/0/0/0	0/2/2/2
4	3ID	A	695	-	-	0/0/0/0	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	694	3ID	C6-C5	-4.55	1.31	1.40
4	A	694	3ID	C4-C9	-2.22	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	695	3ID	C3-C9	2.19	1.61	1.45
4	A	694	3ID	O2-C6	3.39	1.43	1.36
4	A	695	3ID	O2-C6	4.04	1.44	1.36
4	A	694	3ID	O1-C5	4.28	1.45	1.36
4	A	694	3ID	C4-C5	4.77	1.42	1.37
4	A	695	3ID	O1-C5	5.30	1.47	1.36
4	A	694	3ID	C7-C6	6.00	1.43	1.37
4	A	695	3ID	C6-C5	6.35	1.51	1.40
4	A	695	3ID	C7-C6	8.32	1.46	1.37
4	A	695	3ID	C4-C5	8.94	1.46	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	695	3ID	C3-C9-C8	-9.12	98.40	106.20
4	A	694	3ID	C7-C6-C5	-7.64	115.50	119.97
4	A	694	3ID	C2-C3-C9	-5.26	89.49	105.07
4	A	694	3ID	C6-C7-C8	-3.97	114.37	119.99
4	A	694	3ID	C3-C9-C8	-3.94	102.83	106.20
4	A	694	3ID	C7-C8-C9	-3.64	116.48	121.14
4	A	695	3ID	C4-C5-C6	-3.62	117.86	119.97
4	A	695	3ID	C6-C7-C8	-2.89	115.90	119.99
4	A	695	3ID	C7-C6-C5	-2.59	118.46	119.97
4	A	694	3ID	C3-C9-C4	-2.45	127.89	136.63
4	A	695	3ID	C3-C9-C4	-2.09	129.21	136.63
4	A	694	3ID	O2-C6-C7	2.67	127.15	120.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	693	BCT	1	0
4	A	694	3ID	20	0
4	A	695	3ID	1	0

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.