



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:35 PM GMT

PDB ID : 1BIY
Title : STRUCTURE OF DIFERRIC BUFFALO LACTOFERRIN
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Deposited on : 1998-06-21
Resolution : 3.37 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

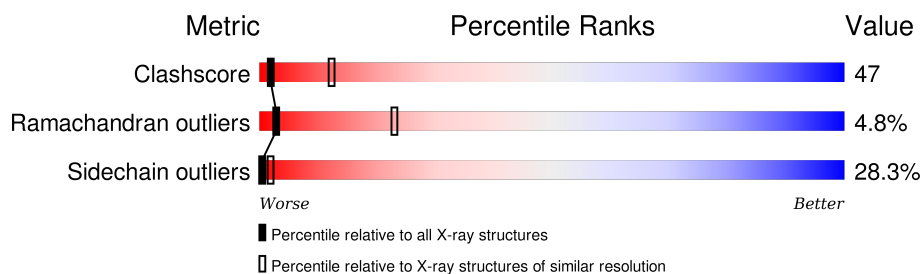
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 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	1158 (3.46-3.30)
Ramachandran outliers	100387	1139 (3.46-3.30)
Sidechain outliers	100360	1138 (3.46-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	689	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5326 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 LACTOFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	689	5316	3340	935	1003	38	0	0	0

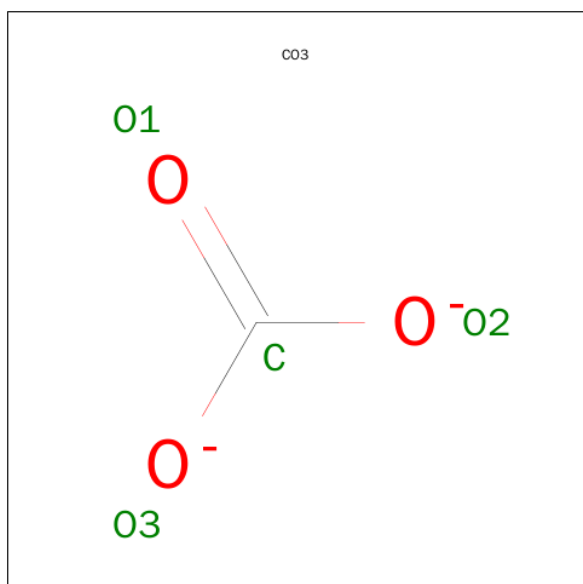
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	LEU	PHE	SEE REMARK 999	UNP O77698
A	303	SER	CYS	SEE REMARK 999	UNP O77698

- 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 CARBONATE ION (three-letter code: CO3) (formula: CO₃).



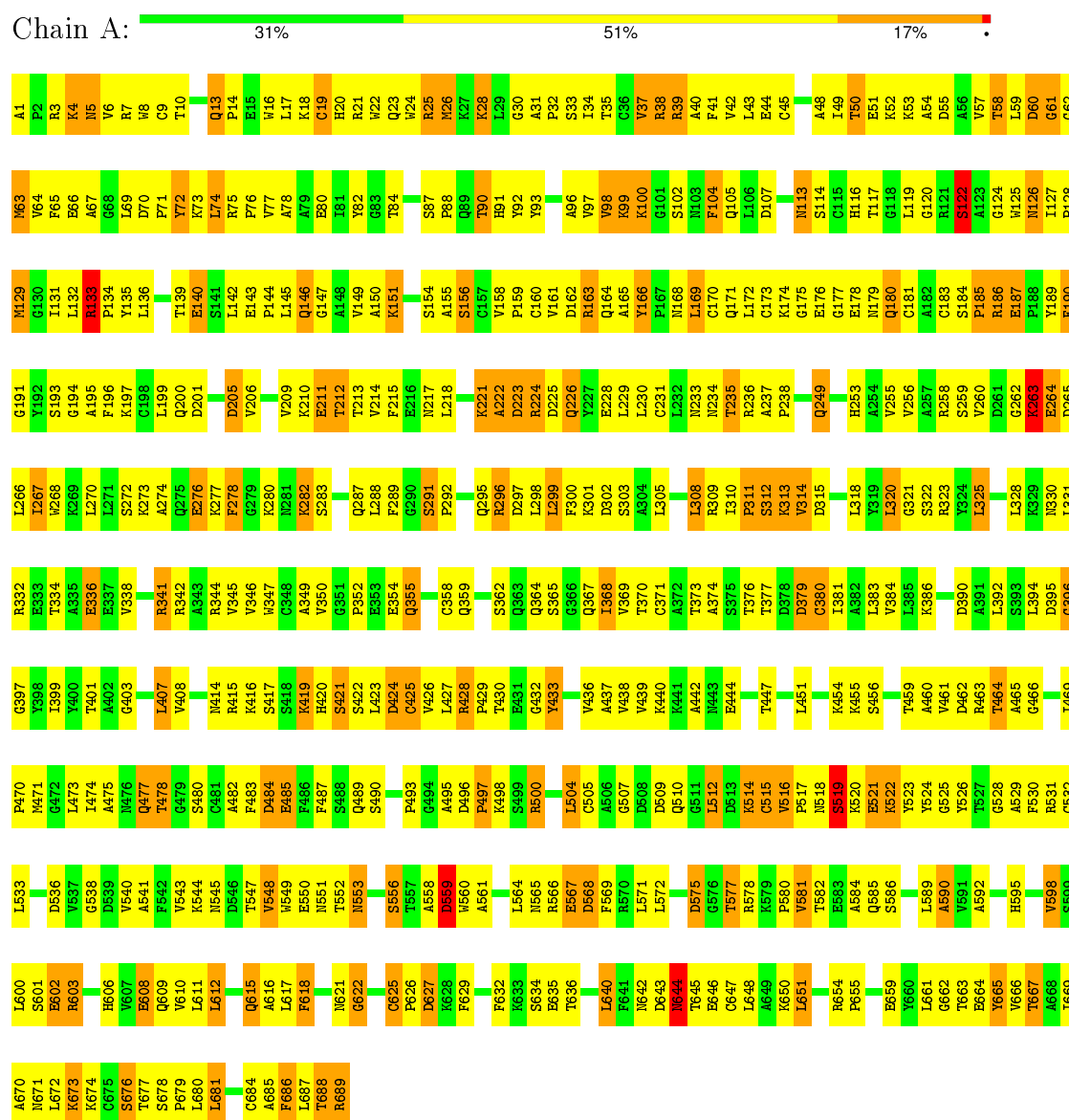
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	A	1	Total	C	O	0	0
			4	1	3		

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 ($RSRZ > 2$). 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: LACTOFERRIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.80 Å 101.44 Å 76.28 Å 90.00° 104.88° 90.00°	Depositor
Resolution (Å)	17.00 – 3.37	Depositor
% Data completeness (in resolution range)	99.0 (17.00-3.37)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5326	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: CO3, 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	0.51	0/5429	0.73	1/7350 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	421	SER	N-CA-C	-5.48	96.22	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	433	TYR	Sidechain

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	5316	0	5216	492	0
2	A	2	0	0	0	0
3	A	8	0	0	0	0
All	All	5326	0	5216	492	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 47.

All (492) 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:41:PHE:HB2	1:A:44:GLU:HG3	1.33	1.09
1:A:678:SER:HB3	1:A:681:LEU:HB2	1.40	1.00
1:A:625:CYS:HB3	1:A:626:PRO:HD3	1.40	1.00
1:A:618:PHE:HB3	1:A:629:PHE:O	1.64	0.98
1:A:414:ASN:HD21	1:A:428:ARG:HD2	1.23	0.96
1:A:31:ALA:HB1	1:A:32:PRO:HD2	1.47	0.96
1:A:200:GLN:HE21	1:A:218:LEU:HD21	1.31	0.95
1:A:455:LYS:HA	1:A:489:GLN:O	1.71	0.91
1:A:147:GLY:HA2	1:A:166:TYR:HE2	1.36	0.88
1:A:113:ASN:H	1:A:113:ASN:HD22	1.15	0.88
1:A:469:ILE:HD13	1:A:590:ALA:HB3	1.56	0.88
1:A:669:ILE:O	1:A:673:LYS:HG2	1.74	0.86
1:A:1:ALA:HB3	1:A:4:LYS:HB2	1.56	0.85
1:A:63:MET:HA	1:A:63:MET:HE3	1.58	0.85
1:A:625:CYS:HB3	1:A:626:PRO:CD	2.06	0.85
1:A:200:GLN:NE2	1:A:218:LEU:HD21	1.92	0.85
1:A:196:PHE:HZ	1:A:218:LEU:HD11	1.41	0.83
1:A:147:GLY:HA2	1:A:166:TYR:CE2	2.12	0.83
1:A:113:ASN:H	1:A:113:ASN:ND2	1.75	0.82
1:A:341:ARG:NH1	1:A:603:ARG:HH21	1.77	0.82
1:A:461:VAL:O	1:A:462:ASP:HB2	1.79	0.81
1:A:9:CYS:HA	1:A:37:VAL:HG22	1.61	0.81
1:A:59:LEU:HB3	1:A:63:MET:HB3	1.63	0.81
1:A:469:ILE:O	1:A:473:LEU:HD12	1.80	0.80
1:A:14:PRO:HB3	1:A:295:GLN:HE22	1.45	0.80
1:A:662:GLY:O	1:A:666:VAL:HG23	1.81	0.80
1:A:451:LEU:HD21	1:A:540:VAL:HG11	1.64	0.79
1:A:341:ARG:HD2	1:A:341:ARG:O	1.82	0.79
1:A:39:ARG:NH1	1:A:48:ALA:HB2	1.96	0.78
1:A:407:LEU:HD12	1:A:598:VAL:HG23	1.65	0.78
1:A:117:THR:HG22	1:A:191:GLY:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LYS:HB3	1:A:504:LEU:HD21	1.66	0.77
1:A:561:ALA:HA	1:A:564:LEU:CD1	2.13	0.77
1:A:211:GLU:HG2	1:A:212:THR:N	2.01	0.76
1:A:211:GLU:HG2	1:A:212:THR:H	1.49	0.76
1:A:438:VAL:HG12	1:A:533:LEU:HD21	1.68	0.76
1:A:461:VAL:HG21	1:A:495:ALA:N	2.01	0.76
1:A:670:ALA:O	1:A:673:LYS:HB2	1.86	0.76
1:A:505:CYS:HB3	1:A:521:GLU:OE1	1.86	0.75
1:A:530:PHE:HE2	1:A:548:VAL:HG13	1.50	0.75
1:A:401:THR:HG23	1:A:681:LEU:HD22	1.68	0.75
1:A:10:THR:HG21	1:A:16:TRP:HA	1.67	0.75
1:A:233:ASN:HB3	1:A:235:THR:HG23	1.66	0.74
1:A:642:ASN:HB3	1:A:644:ASN:ND2	2.01	0.74
1:A:482:ALA:HB1	1:A:485:GLU:HG3	1.68	0.74
1:A:146:GLN:HE21	1:A:146:GLN:H	1.36	0.74
1:A:63:MET:CE	1:A:63:MET:HA	2.18	0.73
1:A:75:ARG:HG2	1:A:76:PRO:HD2	1.70	0.73
1:A:571:LEU:HD11	1:A:581:VAL:HA	1.69	0.73
1:A:7:ARG:HG2	1:A:35:THR:CG2	2.19	0.73
1:A:439:VAL:HG21	1:A:572:LEU:HD21	1.71	0.72
1:A:93:TYR:HD1	1:A:211:GLU:OE1	1.73	0.72
1:A:552:THR:O	1:A:553:ASN:HB2	1.88	0.72
1:A:459:THR:OG1	1:A:466:GLY:HA3	1.89	0.71
1:A:5:ASN:HD21	1:A:7:ARG:HG3	1.55	0.71
1:A:464:THR:HG21	1:A:592:ALA:HB1	1.73	0.71
1:A:276:GLU:O	1:A:282:LYS:HG2	1.91	0.71
1:A:196:PHE:CZ	1:A:218:LEU:HD11	2.25	0.71
1:A:469:ILE:HB	1:A:470:PRO:HD3	1.73	0.70
1:A:119:LEU:HB2	1:A:160:CYS:HB2	1.74	0.70
1:A:263:LYS:HB3	1:A:266:LEU:HD12	1.74	0.70
1:A:58:THR:HG23	1:A:255:VAL:CG2	2.22	0.70
1:A:51:GLU:HB3	1:A:53:LYS:HG3	1.74	0.70
1:A:364:GLN:HG3	1:A:629:PHE:HB2	1.74	0.70
1:A:65:PHE:HB2	1:A:320:LEU:CD1	2.23	0.69
1:A:680:LEU:HG	1:A:680:LEU:O	1.91	0.69
1:A:54:ALA:O	1:A:258:ARG:NH2	2.25	0.69
1:A:41:PHE:HB2	1:A:44:GLU:CG	2.19	0.69
1:A:341:ARG:NH1	1:A:603:ARG:NH2	2.40	0.68
1:A:117:THR:OG1	1:A:124:GLY:HA3	1.92	0.68
1:A:25:ARG:HG3	1:A:28:LYS:NZ	2.09	0.68
1:A:671:ASN:O	1:A:674:LYS:HB3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PRO:HB2	1:A:146:GLN:NE2	2.09	0.68
1:A:58:THR:HG23	1:A:255:VAL:HG23	1.74	0.68
1:A:144:PRO:HG2	1:A:166:TYR:OH	1.94	0.68
1:A:545:ASN:O	1:A:548:VAL:HG23	1.94	0.67
1:A:96:ALA:HB3	1:A:230:LEU:HB2	1.77	0.67
1:A:7:ARG:HB2	1:A:55:ASP:OD2	1.94	0.67
1:A:25:ARG:HG2	1:A:278:PHE:CE1	2.30	0.67
1:A:161:VAL:HG12	1:A:162:ASP:N	2.09	0.67
1:A:354:GLU:HG2	1:A:640:LEU:HD23	1.77	0.67
1:A:129:MET:CE	1:A:132:LEU:HD12	2.25	0.67
1:A:347:TRP:CZ3	1:A:611:LEU:HD11	2.30	0.67
1:A:456:SER:OG	1:A:490:SER:HB3	1.94	0.66
1:A:407:LEU:HD12	1:A:598:VAL:CG2	2.25	0.66
1:A:113:ASN:ND2	1:A:113:ASN:N	2.42	0.66
1:A:221:LYS:O	1:A:224:ARG:N	2.29	0.66
1:A:75:ARG:NH1	1:A:314:VAL:O	2.28	0.66
1:A:6:VAL:HG11	1:A:267:ILE:HG13	1.77	0.66
1:A:374:ALA:HB1	1:A:379:ASP:HB3	1.77	0.66
1:A:7:ARG:HG2	1:A:35:THR:HB	1.76	0.65
1:A:113:ASN:HB3	1:A:172:LEU:HD11	1.78	0.65
1:A:75:ARG:NH2	1:A:312:SER:HA	2.11	0.65
1:A:162:ASP:OD2	1:A:164:GLN:HB3	1.97	0.65
1:A:267:ILE:HG22	1:A:268:TRP:N	2.11	0.65
1:A:114:SER:O	1:A:156:SER:HB3	1.96	0.65
1:A:438:VAL:O	1:A:540:VAL:HG23	1.96	0.65
1:A:464:THR:HG22	1:A:465:ALA:N	2.13	0.64
1:A:98:VAL:HG12	1:A:205:ASP:O	1.97	0.64
1:A:556:SER:HB2	1:A:636:THR:HG21	1.78	0.64
1:A:414:ASN:ND2	1:A:428:ARG:HD2	2.05	0.64
1:A:105:GLN:HE22	1:A:236:ARG:HD2	1.62	0.64
1:A:474:ILE:O	1:A:478:THR:HG23	1.98	0.64
1:A:65:PHE:HB2	1:A:320:LEU:HD11	1.78	0.64
1:A:133:ARG:O	1:A:136:LEU:HB2	1.97	0.64
1:A:146:GLN:NE2	1:A:146:GLN:H	1.96	0.63
1:A:529:ALA:O	1:A:532:CYS:HB3	1.98	0.63
1:A:428:ARG:HG2	1:A:429:PRO:N	2.13	0.63
1:A:483:PHE:HZ	1:A:672:LEU:HD11	1.63	0.63
1:A:76:PRO:HB2	1:A:310:ILE:HD13	1.81	0.63
1:A:642:ASN:HB3	1:A:644:ASN:HD22	1.62	0.63
1:A:289:PHE:O	1:A:302:ASP:HA	1.98	0.63
1:A:530:PHE:CE2	1:A:548:VAL:HG13	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ASN:O	1:A:568:ASP:HB2	1.98	0.62
1:A:173:CYS:HB3	1:A:187:GLU:OE2	2.00	0.62
1:A:22:TRP:CD1	1:A:26:MET:HG2	2.34	0.62
1:A:31:ALA:HB1	1:A:32:PRO:CD	2.26	0.62
1:A:451:LEU:HD21	1:A:540:VAL:CG1	2.30	0.62
1:A:589:LEU:O	1:A:590:ALA:HB2	2.00	0.62
1:A:221:LYS:O	1:A:223:ASP:N	2.33	0.62
1:A:214:VAL:HG13	1:A:215:PHE:H	1.65	0.62
1:A:298:LEU:O	1:A:299:LEU:HB2	2.00	0.61
1:A:97:VAL:HA	1:A:229:LEU:HD23	1.81	0.61
1:A:158:VAL:HG12	1:A:161:VAL:HG23	1.80	0.61
1:A:416:LYS:HD2	1:A:646:GLU:HB2	1.81	0.61
1:A:7:ARG:HG2	1:A:35:THR:CB	2.31	0.61
1:A:75:ARG:CZ	1:A:312:SER:HA	2.31	0.60
1:A:461:VAL:HG23	1:A:493:PRO:O	2.01	0.60
1:A:100:LYS:HA	1:A:228:GLU:OE1	2.01	0.60
1:A:482:ALA:HB1	1:A:485:GLU:CG	2.32	0.60
1:A:214:VAL:HG13	1:A:215:PHE:N	2.16	0.60
1:A:17:LEU:HD21	1:A:21:ARG:HH12	1.67	0.60
1:A:684:CYS:HA	1:A:687:LEU:HB2	1.84	0.59
1:A:561:ALA:HA	1:A:564:LEU:HD11	1.82	0.59
1:A:41:PHE:CB	1:A:44:GLU:HG3	2.23	0.59
1:A:59:LEU:HB3	1:A:63:MET:CB	2.32	0.59
1:A:38:ARG:HD2	1:A:39:ARG:N	2.18	0.59
1:A:392:LEU:N	1:A:392:LEU:HD23	2.18	0.59
1:A:23:GLN:HG3	1:A:34:ILE:HG13	1.84	0.59
1:A:139:THR:HB	1:A:142:LEU:HB3	1.83	0.59
1:A:473:LEU:O	1:A:477:GLN:CG	2.51	0.58
1:A:654:ARG:N	1:A:655:PRO:CD	2.65	0.58
1:A:347:TRP:HZ3	1:A:611:LEU:HD11	1.66	0.58
1:A:531:ARG:HG3	1:A:560:TRP:CD2	2.38	0.58
1:A:49:ILE:O	1:A:258:ARG:NE	2.33	0.58
1:A:650:LYS:HG3	1:A:651:LEU:H	1.67	0.58
1:A:7:ARG:HG2	1:A:35:THR:HG21	1.84	0.58
1:A:97:VAL:HG22	1:A:229:LEU:HD21	1.85	0.58
1:A:17:LEU:HD21	1:A:21:ARG:NH1	2.18	0.58
1:A:544:LYS:O	1:A:547:THR:HB	2.02	0.58
1:A:23:GLN:HA	1:A:34:ILE:HD11	1.86	0.58
1:A:39:ARG:CZ	1:A:48:ALA:HB2	2.34	0.58
1:A:490:SER:HA	1:A:504:LEU:HD22	1.86	0.57
1:A:145:LEU:O	1:A:149:VAL:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:SER:OG	1:A:116:HIS:HE1	1.86	0.57
1:A:654:ARG:NH1	1:A:654:ARG:HB2	2.18	0.57
1:A:127:ILE:O	1:A:131:ILE:HG12	2.04	0.57
1:A:308:LEU:HD13	1:A:686:PHE:HE2	1.69	0.57
1:A:122:SER:HA	1:A:126:ASN:HB2	1.86	0.57
1:A:18:LYS:HG2	1:A:299:LEU:HD12	1.85	0.57
1:A:51:GLU:O	1:A:53:LYS:HG3	2.05	0.57
1:A:295:GLN:C	1:A:296:ARG:HG2	2.25	0.57
1:A:187:GLU:O	1:A:190:PHE:HB3	2.05	0.57
1:A:19:CYS:SG	1:A:20:HIS:HD2	2.28	0.57
1:A:473:LEU:O	1:A:477:GLN:HG2	2.04	0.57
1:A:57:VAL:HG22	1:A:58:THR:H	1.69	0.57
1:A:349:ALA:O	1:A:373:THR:HG23	2.05	0.57
1:A:634:SER:O	1:A:635:GLU:HB2	2.04	0.57
1:A:13:GLN:N	1:A:14:PRO:HD2	2.20	0.57
1:A:175:GLY:O	1:A:180:GLN:HB2	2.05	0.57
1:A:25:ARG:HG3	1:A:28:LYS:HZ1	1.69	0.57
1:A:113:ASN:HA	1:A:155:ALA:O	2.05	0.56
1:A:177:GLY:C	1:A:179:ASN:N	2.56	0.56
1:A:484:ASP:O	1:A:500:ARG:HD2	2.04	0.56
1:A:143:GLU:HB2	1:A:144:PRO:HD2	1.87	0.56
1:A:77:VAL:HB	1:A:255:VAL:O	2.06	0.56
1:A:102:SER:HB2	1:A:236:ARG:HH22	1.70	0.56
1:A:163:ARG:HA	1:A:166:TYR:O	2.04	0.56
1:A:156:SER:O	1:A:169:LEU:O	2.22	0.56
1:A:686:PHE:C	1:A:686:PHE:CD1	2.78	0.56
1:A:330:ASN:N	1:A:330:ASN:HD22	2.01	0.56
1:A:23:GLN:CA	1:A:34:ILE:HD11	2.35	0.56
1:A:184:SER:O	1:A:186:ARG:N	2.39	0.56
1:A:618:PHE:CD2	1:A:629:PHE:HD2	2.24	0.55
1:A:526:TYR:CE1	1:A:544:LYS:HB3	2.41	0.55
1:A:140:GLU:HG3	1:A:334:THR:HB	1.87	0.55
1:A:627:ASP:N	1:A:627:ASP:OD1	2.31	0.55
1:A:368:ILE:HG22	1:A:369:VAL:HG23	1.89	0.55
1:A:338:VAL:HG13	1:A:342:ARG:NH1	2.22	0.55
1:A:505:CYS:O	1:A:514:LYS:HD3	2.07	0.55
1:A:377:THR:O	1:A:381:ILE:HD12	2.07	0.55
1:A:128:PRO:O	1:A:132:LEU:HG	2.07	0.55
1:A:291:SER:OG	1:A:302:ASP:OD1	2.25	0.55
1:A:370:THR:HG22	1:A:371:CYS:N	2.21	0.55
1:A:143:GLU:OE1	1:A:151:LYS:NZ	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TRP:NE1	1:A:26:MET:HG2	2.22	0.55
1:A:362:SER:O	1:A:365:SER:OG	2.19	0.55
1:A:49:ILE:N	1:A:54:ALA:HB3	2.22	0.54
1:A:288:LEU:HD11	1:A:300:PHE:HE2	1.72	0.54
1:A:133:ARG:HB3	1:A:134:PRO:HD3	1.89	0.54
1:A:521:GLU:OE2	1:A:523:TYR:N	2.33	0.54
1:A:464:THR:HG21	1:A:592:ALA:CB	2.37	0.54
1:A:315:ASP:OD1	1:A:318:LEU:HB2	2.07	0.54
1:A:437:ALA:HB3	1:A:572:LEU:HB2	1.88	0.54
1:A:558:ALA:O	1:A:560:TRP:N	2.40	0.54
1:A:665:TYR:CE1	1:A:669:ILE:HD11	2.43	0.54
1:A:618:PHE:CD1	1:A:618:PHE:N	2.76	0.54
1:A:19:CYS:SG	1:A:20:HIS:N	2.79	0.54
1:A:262:GLY:O	1:A:264:GLU:N	2.41	0.53
1:A:14:PRO:HB3	1:A:295:GLN:NE2	2.21	0.53
1:A:14:PRO:HG3	1:A:295:GLN:OE1	2.09	0.53
1:A:49:ILE:HA	1:A:54:ALA:HB3	1.91	0.53
1:A:650:LYS:HG3	1:A:651:LEU:N	2.23	0.53
1:A:346:VAL:H	1:A:390:ASP:HB2	1.74	0.53
1:A:38:ARG:HH22	1:A:186:ARG:HH22	1.57	0.53
1:A:439:VAL:CG2	1:A:572:LEU:HD21	2.36	0.53
1:A:177:GLY:C	1:A:179:ASN:H	2.11	0.53
1:A:32:PRO:HG2	1:A:270:LEU:HB2	1.89	0.53
1:A:5:ASN:ND2	1:A:35:THR:HB	2.24	0.52
1:A:673:LYS:O	1:A:676:SER:O	2.26	0.52
1:A:38:ARG:NH2	1:A:186:ARG:HH22	2.07	0.52
1:A:654:ARG:HH11	1:A:654:ARG:HB2	1.72	0.52
1:A:362:SER:HA	1:A:369:VAL:O	2.08	0.52
1:A:180:GLN:HG2	1:A:181:CYS:N	2.22	0.52
1:A:114:SER:OG	1:A:116:HIS:CE1	2.62	0.52
1:A:380:CYS:HB3	1:A:392:LEU:HD13	1.91	0.52
1:A:370:THR:CG2	1:A:371:CYS:N	2.71	0.52
1:A:678:SER:CB	1:A:681:LEU:HB2	2.24	0.52
1:A:57:VAL:HG22	1:A:58:THR:N	2.23	0.52
1:A:7:ARG:CG	1:A:35:THR:HB	2.40	0.52
1:A:114:SER:OG	1:A:156:SER:HB3	2.09	0.52
1:A:455:LYS:HB2	1:A:538:GLY:HA2	1.92	0.52
1:A:96:ALA:CB	1:A:230:LEU:HB2	2.40	0.52
1:A:73:LYS:HG2	1:A:259:SER:HB2	1.92	0.52
1:A:19:CYS:O	1:A:22:TRP:HB3	2.10	0.52
1:A:394:LEU:HD12	1:A:598:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LYS:HD2	1:A:536:ASP:OD1	2.10	0.52
1:A:217:ASN:O	1:A:218:LEU:HD23	2.10	0.51
1:A:550:GLU:OE2	1:A:644:ASN:HB3	2.10	0.51
1:A:311:PRO:O	1:A:313:LYS:N	2.43	0.51
1:A:330:ASN:N	1:A:330:ASN:ND2	2.58	0.51
1:A:336:GLU:OE1	1:A:336:GLU:N	2.43	0.51
1:A:347:TRP:CE2	1:A:392:LEU:HA	2.45	0.51
1:A:292:PRO:HD2	1:A:298:LEU:HD12	1.93	0.51
1:A:107:ASP:OD1	1:A:107:ASP:N	2.44	0.51
1:A:196:PHE:O	1:A:197:LYS:C	2.49	0.51
1:A:263:LYS:O	1:A:267:ILE:HD12	2.11	0.51
1:A:147:GLY:O	1:A:150:ALA:HB3	2.11	0.51
1:A:469:ILE:CD1	1:A:590:ALA:HB3	2.33	0.51
1:A:10:THR:OG1	1:A:38:ARG:HG2	2.09	0.51
1:A:60:ASP:O	1:A:61:GLY:C	2.49	0.51
1:A:451:LEU:O	1:A:454:LYS:HG2	2.09	0.51
1:A:522:LYS:HE2	1:A:523:TYR:CZ	2.46	0.51
1:A:49:ILE:CA	1:A:54:ALA:HB3	2.40	0.51
1:A:350:VAL:HG12	1:A:350:VAL:O	2.09	0.51
1:A:237:ALA:HB1	1:A:238:PRO:HD2	1.91	0.51
1:A:603:ARG:NH1	1:A:606:HIS:CD2	2.79	0.51
1:A:184:SER:C	1:A:186:ARG:N	2.64	0.51
1:A:205:ASP:OD1	1:A:205:ASP:N	2.44	0.51
1:A:184:SER:C	1:A:186:ARG:H	2.14	0.51
1:A:518:ASN:OD1	1:A:520:LYS:HB2	2.11	0.51
1:A:493:PRO:HA	1:A:515:CYS:SG	2.51	0.50
1:A:416:LYS:CD	1:A:646:GLU:HB2	2.41	0.50
1:A:603:ARG:NH1	1:A:606:HIS:HD2	2.10	0.50
1:A:490:SER:CA	1:A:504:LEU:HD22	2.40	0.50
1:A:611:LEU:HD13	1:A:648:LEU:HD13	1.94	0.50
1:A:165:ALA:HB3	1:A:166:TYR:CD1	2.46	0.50
1:A:665:TYR:HD1	1:A:665:TYR:C	2.15	0.50
1:A:6:VAL:CG1	1:A:267:ILE:HG13	2.40	0.50
1:A:145:LEU:C	1:A:147:GLY:N	2.64	0.50
1:A:63:MET:HE3	1:A:66:GLU:HB2	1.92	0.50
1:A:533:LEU:HB2	1:A:541:ALA:HB2	1.93	0.50
1:A:611:LEU:O	1:A:615:GLN:HB3	2.12	0.50
1:A:459:THR:O	1:A:460:ALA:HB2	2.12	0.50
1:A:18:LYS:HE2	1:A:299:LEU:HB2	1.94	0.50
1:A:91:HIS:CD2	1:A:249:GLN:HG2	2.45	0.50
1:A:567:GLU:C	1:A:569:PHE:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:VAL:HG12	1:A:533:LEU:CD2	2.40	0.50
1:A:31:ALA:O	1:A:33:SER:N	2.45	0.49
1:A:456:SER:OG	1:A:487:PHE:CD2	2.65	0.49
1:A:377:THR:HG22	1:A:381:ILE:HD12	1.95	0.49
1:A:456:SER:HG	1:A:487:PHE:HD2	1.53	0.49
1:A:170:CYS:O	1:A:173:CYS:HB2	2.13	0.49
1:A:616:ALA:O	1:A:622:GLY:HA2	2.12	0.49
1:A:551:ASN:O	1:A:561:ALA:HB1	2.12	0.49
1:A:60:ASP:HA	1:A:253:HIS:CD2	2.48	0.49
1:A:345:VAL:HG23	1:A:610:VAL:HG21	1.94	0.49
1:A:185:PRO:HA	1:A:190:PHE:HD2	1.76	0.49
1:A:58:THR:HG23	1:A:255:VAL:HG22	1.94	0.49
1:A:221:LYS:O	1:A:222:ALA:C	2.51	0.49
1:A:313:LYS:HG3	1:A:679:PRO:HB2	1.94	0.49
1:A:665:TYR:CD1	1:A:665:TYR:C	2.85	0.49
1:A:5:ASN:HB2	1:A:33:SER:O	2.13	0.49
1:A:456:SER:OG	1:A:490:SER:CB	2.60	0.49
1:A:146:GLN:HE21	1:A:146:GLN:N	2.07	0.49
1:A:161:VAL:HG12	1:A:162:ASP:H	1.75	0.49
1:A:100:LYS:HD3	1:A:228:GLU:HG3	1.94	0.49
1:A:315:ASP:N	1:A:315:ASP:OD1	2.39	0.49
1:A:87:SER:N	1:A:88:PRO:HD3	2.28	0.49
1:A:341:ARG:HD2	1:A:341:ARG:C	2.30	0.48
1:A:161:VAL:CG1	1:A:162:ASP:N	2.74	0.48
1:A:687:LEU:O	1:A:688:THR:C	2.52	0.48
1:A:341:ARG:HH12	1:A:390:ASP:CG	2.15	0.48
1:A:461:VAL:HG21	1:A:495:ALA:H	1.72	0.48
1:A:38:ARG:NH1	1:A:39:ARG:O	2.43	0.48
1:A:228:GLU:O	1:A:229:LEU:HD23	2.12	0.48
1:A:82:TYR:HE2	1:A:92:TYR:HD2	1.61	0.48
1:A:168:ASN:HA	1:A:171:GLN:HB2	1.94	0.48
1:A:571:LEU:CD1	1:A:584:ALA:HB2	2.44	0.48
1:A:155:ALA:HA	1:A:168:ASN:O	2.13	0.48
1:A:615:GLN:OE1	1:A:648:LEU:HB2	2.14	0.48
1:A:181:CYS:CA	1:A:187:GLU:HG3	2.43	0.48
1:A:399:ILE:O	1:A:403:GLY:N	2.38	0.48
1:A:399:ILE:HD12	1:A:661:LEU:HD21	1.96	0.48
1:A:40:ALA:O	1:A:184:SER:HB3	2.13	0.48
1:A:97:VAL:HA	1:A:229:LEU:CD2	2.44	0.48
1:A:193:SER:O	1:A:196:PHE:N	2.44	0.48
1:A:196:PHE:O	1:A:199:LEU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ARG:HB3	1:A:278:PHE:CZ	2.49	0.47
1:A:7:ARG:O	1:A:55:ASP:HB2	2.14	0.47
1:A:14:PRO:CB	1:A:295:GLN:HE22	2.23	0.47
1:A:100:LYS:HG3	1:A:226:GLN:HA	1.97	0.47
1:A:57:VAL:O	1:A:255:VAL:HG13	2.13	0.47
1:A:507:GLY:HA2	1:A:521:GLU:HA	1.96	0.47
1:A:355:GLN:O	1:A:359:GLN:HG3	2.14	0.47
1:A:380:CYS:O	1:A:384:VAL:HG23	2.15	0.47
1:A:617:LEU:HB2	1:A:618:PHE:CE1	2.50	0.47
1:A:144:PRO:HB2	1:A:146:GLN:HE21	1.80	0.47
1:A:354:GLU:CG	1:A:640:LEU:HD23	2.45	0.47
1:A:82:TYR:HE2	1:A:92:TYR:CD2	2.33	0.47
1:A:422:SER:O	1:A:423:LEU:C	2.52	0.47
1:A:589:LEU:HD23	1:A:589:LEU:N	2.28	0.47
1:A:102:SER:HB2	1:A:236:ARG:NH2	2.29	0.47
1:A:105:GLN:HG3	1:A:234:ASN:O	2.15	0.47
1:A:185:PRO:HA	1:A:190:PHE:CD2	2.50	0.47
1:A:77:VAL:HG11	1:A:267:ILE:HG21	1.96	0.47
1:A:483:PHE:C	1:A:485:GLU:N	2.67	0.47
1:A:288:LEU:HD11	1:A:300:PHE:CE2	2.49	0.46
1:A:470:PRO:O	1:A:474:ILE:HD12	2.16	0.46
1:A:352:PRO:HG3	1:A:520:LYS:HD2	1.97	0.46
1:A:119:LEU:CB	1:A:160:CYS:HB2	2.44	0.46
1:A:5:ASN:HD21	1:A:35:THR:HB	1.81	0.46
1:A:75:ARG:O	1:A:256:VAL:HA	2.15	0.46
1:A:7:ARG:CB	1:A:55:ASP:OD2	2.63	0.46
1:A:482:ALA:CB	1:A:485:GLU:HG3	2.43	0.46
1:A:132:LEU:O	1:A:133:ARG:C	2.53	0.46
1:A:69:LEU:C	1:A:71:PRO:HD2	2.35	0.46
1:A:199:LEU:HG	1:A:199:LEU:O	2.16	0.46
1:A:60:ASP:HB2	1:A:253:HIS:CE1	2.50	0.46
1:A:91:HIS:HD2	1:A:249:GLN:HG2	1.80	0.46
1:A:7:ARG:N	1:A:55:ASP:OD2	2.40	0.46
1:A:469:ILE:CB	1:A:470:PRO:HD3	2.43	0.46
1:A:65:PHE:CD1	1:A:65:PHE:C	2.88	0.46
1:A:67:ALA:O	1:A:72:TYR:O	2.34	0.46
1:A:213:THR:O	1:A:217:ASN:ND2	2.49	0.46
1:A:392:LEU:HD11	1:A:394:LEU:HD21	1.98	0.46
1:A:665:TYR:CE1	1:A:669:ILE:CG1	2.98	0.46
1:A:233:ASN:O	1:A:234:ASN:HB2	2.16	0.46
1:A:438:VAL:HG12	1:A:439:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.77	0.45
1:A:455:LYS:HB3	1:A:504:LEU:CD2	2.40	0.45
1:A:166:TYR:CD1	1:A:166:TYR:N	2.85	0.45
1:A:407:LEU:C	1:A:408:VAL:HG13	2.37	0.45
1:A:5:ASN:HD21	1:A:7:ARG:CG	2.27	0.45
1:A:461:VAL:CG2	1:A:495:ALA:H	2.30	0.45
1:A:277:LYS:O	1:A:282:LYS:HB3	2.16	0.45
1:A:523:TYR:HA	1:A:528:GLY:O	2.16	0.45
1:A:22:TRP:HZ2	1:A:274:ALA:HB2	1.82	0.45
1:A:377:THR:HG22	1:A:381:ILE:CD1	2.46	0.45
1:A:439:VAL:HG13	1:A:540:VAL:HG23	1.99	0.45
1:A:181:CYS:N	1:A:187:GLU:HG3	2.31	0.45
1:A:308:LEU:HD13	1:A:686:PHE:CE2	2.49	0.45
1:A:561:ALA:HA	1:A:564:LEU:CG	2.45	0.45
1:A:483:PHE:C	1:A:485:GLU:H	2.19	0.45
1:A:282:LYS:HA	1:A:282:LYS:HE3	1.98	0.45
1:A:396:GLY:O	1:A:399:ILE:N	2.50	0.45
1:A:504:LEU:N	1:A:504:LEU:HD13	2.31	0.45
1:A:98:VAL:HG13	1:A:206:VAL:HG23	1.99	0.45
1:A:125:TRP:CH2	1:A:149:VAL:HG11	2.52	0.45
1:A:165:ALA:HB3	1:A:166:TYR:CE1	2.52	0.45
1:A:38:ARG:HD2	1:A:39:ARG:H	1.81	0.45
1:A:407:LEU:O	1:A:408:VAL:CG1	2.65	0.45
1:A:97:VAL:O	1:A:206:VAL:HG23	2.17	0.45
1:A:544:LYS:HG2	1:A:547:THR:OG1	2.17	0.45
1:A:681:LEU:HD13	1:A:681:LEU:HA	1.63	0.45
1:A:561:ALA:HA	1:A:564:LEU:HG	1.99	0.45
1:A:571:LEU:HD11	1:A:584:ALA:HB2	1.98	0.44
1:A:93:TYR:CD1	1:A:211:GLU:OE1	2.63	0.44
1:A:314:VAL:O	1:A:314:VAL:CG2	2.66	0.44
1:A:16:TRP:CD1	1:A:38:ARG:HG2	2.52	0.44
1:A:221:LYS:C	1:A:223:ASP:N	2.70	0.44
1:A:469:ILE:CB	1:A:470:PRO:CD	2.96	0.44
1:A:469:ILE:HB	1:A:470:PRO:CD	2.42	0.44
1:A:643:ASP:C	1:A:645:THR:H	2.21	0.44
1:A:571:LEU:CD1	1:A:581:VAL:HA	2.42	0.44
1:A:685:ALA:O	1:A:688:THR:OG1	2.35	0.44
1:A:522:LYS:HE3	1:A:531:ARG:NH1	2.33	0.44
1:A:602:GLU:H	1:A:602:GLU:CD	2.19	0.44
1:A:558:ALA:C	1:A:560:TRP:H	2.20	0.44
1:A:17:LEU:HD12	1:A:17:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:CYS:CB	1:A:626:PRO:CD	2.86	0.44
1:A:667:THR:O	1:A:670:ALA:HB3	2.18	0.44
1:A:42:VAL:HG22	1:A:42:VAL:O	2.18	0.44
1:A:575:ASP:HB2	1:A:577:THR:CG2	2.47	0.44
1:A:469:ILE:N	1:A:470:PRO:HD2	2.32	0.43
1:A:267:ILE:CG2	1:A:268:TRP:N	2.80	0.43
1:A:61:GLY:O	1:A:64:VAL:HB	2.18	0.43
1:A:612:LEU:HA	1:A:612:LEU:HD22	1.81	0.43
1:A:428:ARG:HG2	1:A:429:PRO:CD	2.49	0.43
1:A:516:VAL:O	1:A:516:VAL:CG1	2.66	0.43
1:A:425:CYS:O	1:A:427:LEU:N	2.51	0.43
1:A:512:LEU:HG	1:A:512:LEU:H	1.59	0.43
1:A:25:ARG:HG3	1:A:28:LYS:HZ2	1.82	0.43
1:A:686:PHE:CZ	1:A:689:ARG:NH1	2.86	0.43
1:A:519:SER:O	1:A:520:LYS:C	2.54	0.43
1:A:159:PRO:HG3	1:A:190:PHE:HA	2.00	0.43
1:A:52:LYS:HA	1:A:258:ARG:NH2	2.33	0.43
1:A:104:PHE:C	1:A:104:PHE:CD1	2.91	0.43
1:A:34:ILE:CG2	1:A:270:LEU:HD11	2.48	0.43
1:A:161:VAL:CG1	1:A:162:ASP:H	2.31	0.43
1:A:221:LYS:HD3	1:A:225:ASP:OD1	2.18	0.43
1:A:74:LEU:HB3	1:A:256:VAL:HB	2.01	0.43
1:A:159:PRO:O	1:A:160:CYS:HB2	2.18	0.43
1:A:419:LYS:HG3	1:A:420:HIS:CE1	2.53	0.43
1:A:471:MET:O	1:A:475:ALA:HB2	2.18	0.43
1:A:416:LYS:NZ	1:A:646:GLU:OE2	2.39	0.43
1:A:550:GLU:C	1:A:551:ASN:ND2	2.72	0.43
1:A:552:THR:O	1:A:553:ASN:CB	2.61	0.43
1:A:147:GLY:CA	1:A:166:TYR:CE2	2.92	0.43
1:A:665:TYR:O	1:A:665:TYR:HD1	2.01	0.43
1:A:384:VAL:HG11	1:A:407:LEU:HD11	2.01	0.43
1:A:120:GLY:O	1:A:126:ASN:ND2	2.51	0.43
1:A:233:ASN:CB	1:A:235:THR:HG23	2.45	0.42
1:A:78:ALA:N	1:A:310:ILE:HD12	2.34	0.42
1:A:61:GLY:O	1:A:62:GLY:C	2.57	0.42
1:A:496:ASP:C	1:A:498:LYS:H	2.22	0.42
1:A:632:PHE:O	1:A:643:ASP:HA	2.19	0.42
1:A:211:GLU:CG	1:A:212:THR:N	2.77	0.42
1:A:423:LEU:HD23	1:A:424:ASP:N	2.35	0.42
1:A:456:SER:H	1:A:490:SER:HB3	1.85	0.42
1:A:483:PHE:CZ	1:A:672:LEU:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ALA:HB3	1:A:209:VAL:CG1	2.49	0.42
1:A:589:LEU:O	1:A:590:ALA:CB	2.66	0.42
1:A:8:TRP:N	1:A:35:THR:O	2.47	0.42
1:A:321:GLY:O	1:A:325:LEU:HB2	2.19	0.42
1:A:663:THR:O	1:A:667:THR:OG1	2.36	0.42
1:A:173:CYS:CB	1:A:187:GLU:OE2	2.65	0.42
1:A:50:THR:HG21	1:A:72:TYR:HB3	2.01	0.42
1:A:496:ASP:O	1:A:498:LYS:N	2.50	0.42
1:A:189:TYR:HA	1:A:194:GLY:O	2.19	0.42
1:A:229:LEU:HA	1:A:229:LEU:HD23	1.77	0.42
1:A:76:PRO:O	1:A:310:ILE:HG21	2.19	0.42
1:A:433:TYR:CZ	1:A:526:TYR:OH	2.73	0.42
1:A:82:TYR:CE2	1:A:92:TYR:HD2	2.38	0.42
1:A:428:ARG:CG	1:A:429:PRO:HD2	2.50	0.42
1:A:7:ARG:HA	1:A:35:THR:O	2.19	0.42
1:A:642:ASN:HB2	1:A:645:THR:OG1	2.20	0.41
1:A:526:TYR:CD2	1:A:544:LYS:HE2	2.55	0.41
1:A:559:ASP:C	1:A:559:ASP:OD1	2.58	0.41
1:A:383:LEU:HA	1:A:383:LEU:HD23	1.71	0.41
1:A:618:PHE:CD2	1:A:629:PHE:O	2.74	0.41
1:A:231:CYS:C	1:A:233:ASN:N	2.73	0.41
1:A:571:LEU:HD21	1:A:581:VAL:HG12	2.03	0.41
1:A:358:CYS:C	1:A:371:CYS:SG	2.98	0.41
1:A:438:VAL:O	1:A:540:VAL:HA	2.19	0.41
1:A:408:VAL:HG23	1:A:408:VAL:O	2.19	0.41
1:A:496:ASP:HA	1:A:497:PRO:HD2	1.88	0.41
1:A:436:VAL:HG22	1:A:543:VAL:O	2.21	0.41
1:A:549:TRP:CE3	1:A:566:ARG:NH1	2.89	0.41
1:A:159:PRO:O	1:A:160:CYS:CB	2.68	0.41
1:A:608:GLU:OE1	1:A:650:LYS:HE3	2.20	0.41
1:A:98:VAL:HG11	1:A:104:PHE:CE1	2.56	0.41
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.88	0.41
1:A:122:SER:O	1:A:126:ASN:HB2	2.21	0.41
1:A:618:PHE:CB	1:A:629:PHE:O	2.52	0.41
1:A:553:ASN:ND2	1:A:566:ARG:HB2	2.35	0.41
1:A:459:THR:HG1	1:A:466:GLY:HA3	1.81	0.41
1:A:454:LYS:HD3	1:A:454:LYS:HA	1.76	0.41
1:A:521:GLU:O	1:A:524:TYR:HB3	2.21	0.41
1:A:181:CYS:HA	1:A:187:GLU:HG3	2.03	0.41
1:A:116:HIS:HB2	1:A:158:VAL:HG22	2.02	0.41
1:A:438:VAL:CG1	1:A:533:LEU:HD21	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ARG:N	1:A:655:PRO:HD3	2.35	0.40
1:A:80:GLU:O	1:A:90:THR:HG22	2.20	0.40
1:A:678:SER:O	1:A:681:LEU:N	2.53	0.40
1:A:99:LYS:HE3	1:A:199:LEU:O	2.21	0.40
1:A:266:LEU:H	1:A:266:LEU:HG	1.76	0.40
1:A:64:VAL:HG12	1:A:65:PHE:N	2.36	0.40
1:A:567:GLU:C	1:A:569:PHE:N	2.75	0.40
1:A:504:LEU:N	1:A:504:LEU:CD1	2.83	0.40
1:A:52:LYS:HA	1:A:258:ARG:HH21	1.87	0.40
1:A:395:ASP:HA	1:A:595:HIS:CG	2.56	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	687/689 (100%)	553 (80%)	101 (15%)	33 (5%)	3	23

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	263	LYS
1	A	311	PRO
1	A	464	THR
1	A	553	ASN
1	A	559	ASP
1	A	30	GLY
1	A	122	SER
1	A	222	ALA
1	A	312	SER
1	A	320	LEU

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Mol	Chain	Res	Type
1	A	397	GLY
1	A	425	CYS
1	A	568	ASP
1	A	644	ASN
1	A	201	ASP
1	A	396	GLY
1	A	426	VAL
1	A	497	PRO
1	A	299	LEU
1	A	519	SER
1	A	590	ALA
1	A	622	GLY
1	A	133	ARG
1	A	297	ASP
1	A	442	ALA
1	A	625	CYS
1	A	432	GLY
1	A	517	PRO
1	A	525	GLY
1	A	61	GLY
1	A	581	VAL
1	A	185	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	569/569 (100%)	408 (72%)	161 (28%)	0 2

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	LYS
1	A	5	ASN
1	A	13	GLN

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Mol	Chain	Res	Type
1	A	19	CYS
1	A	24	TRP
1	A	25	ARG
1	A	26	MET
1	A	28	LYS
1	A	37	VAL
1	A	38	ARG
1	A	39	ARG
1	A	43	LEU
1	A	45	CYS
1	A	50	THR
1	A	58	THR
1	A	60	ASP
1	A	63	MET
1	A	70	ASP
1	A	72	TYR
1	A	74	LEU
1	A	84	THR
1	A	90	THR
1	A	98	VAL
1	A	99	LYS
1	A	100	LYS
1	A	104	PHE
1	A	113	ASN
1	A	122	SER
1	A	129	MET
1	A	133	ARG
1	A	135	TYR
1	A	140	GLU
1	A	146	GLN
1	A	151	LYS
1	A	154	SER
1	A	156	SER
1	A	163	ARG
1	A	166	TYR
1	A	169	LEU
1	A	174	LYS
1	A	176	GLU
1	A	178	GLU
1	A	180	GLN
1	A	183	CYS
1	A	186	ARG

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Mol	Chain	Res	Type
1	A	187	GLU
1	A	190	PHE
1	A	205	ASP
1	A	210	LYS
1	A	211	GLU
1	A	212	THR
1	A	221	LYS
1	A	223	ASP
1	A	224	ARG
1	A	226	GLN
1	A	235	THR
1	A	249	GLN
1	A	260	VAL
1	A	263	LYS
1	A	264	GLU
1	A	265	ASP
1	A	267	ILE
1	A	272	SER
1	A	273	LYS
1	A	276	GLU
1	A	278	PHE
1	A	280	LYS
1	A	282	LYS
1	A	283	SER
1	A	287	GLN
1	A	291	SER
1	A	296	ARG
1	A	301	LYS
1	A	303	SER
1	A	305	LEU
1	A	308	LEU
1	A	309	ARG
1	A	313	LYS
1	A	314	VAL
1	A	322	SER
1	A	323	ARG
1	A	325	LEU
1	A	328	LEU
1	A	331	LEU
1	A	332	ARG
1	A	336	GLU
1	A	341	ARG

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Mol	Chain	Res	Type
1	A	344	ARG
1	A	355	GLN
1	A	367	GLN
1	A	368	ILE
1	A	376	THR
1	A	379	ASP
1	A	380	CYS
1	A	386	LYS
1	A	407	LEU
1	A	415	ARG
1	A	417	SER
1	A	419	LYS
1	A	421	SER
1	A	424	ASP
1	A	428	ARG
1	A	430	THR
1	A	444	GLU
1	A	447	THR
1	A	463	ARG
1	A	477	GLN
1	A	478	THR
1	A	480	SER
1	A	484	ASP
1	A	485	GLU
1	A	500	ARG
1	A	504	LEU
1	A	509	ASP
1	A	510	GLN
1	A	512	LEU
1	A	514	LYS
1	A	515	CYS
1	A	516	VAL
1	A	519	SER
1	A	521	GLU
1	A	522	LYS
1	A	548	VAL
1	A	556	SER
1	A	559	ASP
1	A	567	GLU
1	A	575	ASP
1	A	577	THR
1	A	578	ARG

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Mol	Chain	Res	Type
1	A	580	PRO
1	A	582	THR
1	A	585	GLN
1	A	586	SER
1	A	598	VAL
1	A	600	LEU
1	A	601	SER
1	A	602	GLU
1	A	603	ARG
1	A	608	GLU
1	A	609	GLN
1	A	612	LEU
1	A	615	GLN
1	A	618	PHE
1	A	621	ASN
1	A	627	ASP
1	A	640	LEU
1	A	644	ASN
1	A	647	CYS
1	A	651	LEU
1	A	659	GLU
1	A	664	GLU
1	A	665	TYR
1	A	667	THR
1	A	673	LYS
1	A	676	SER
1	A	677	THR
1	A	681	LEU
1	A	686	PHE
1	A	688	THR
1	A	689	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	20	HIS
1	A	91	HIS
1	A	105	GLN
1	A	110	GLN
1	A	113	ASN
1	A	116	HIS

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Mol	Chain	Res	Type
1	A	126	ASN
1	A	146	GLN
1	A	200	GLN
1	A	217	ASN
1	A	226	GLN
1	A	330	ASN
1	A	363	GLN
1	A	414	ASN
1	A	551	ASN
1	A	553	ASN
1	A	585	GLN
1	A	588	HIS
1	A	606	HIS
1	A	609	GLN
1	A	621	ASN
1	A	644	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	CO3	A	692	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	A	693	2	0,3,3	0.00	-	0,3,3	0.00	-

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	CO3	A	692	2	-	0/0/0/0	0/0/0/0
3	CO3	A	693	2	-	0/0/0/0	0/0/0/0

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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