



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2018 – 02:12 AM EST

PDB ID : 1BIH
Title : CRYSTAL STRUCTURE OF THE INSECT IMMUNE PROTEIN
HEMOLIN: A NEW DOMAIN ARRANGEMENT WITH IMPLICATIONS
FOR HOMOPHILIC ADHESION
Authors : Su, X.-D.; Gastinel, L.N.; Vaughn, D.E.; Faye, I.; Poon, P.; Bjorkman, P.J.
Deposited on : 1998-06-17
Resolution : 3.10 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

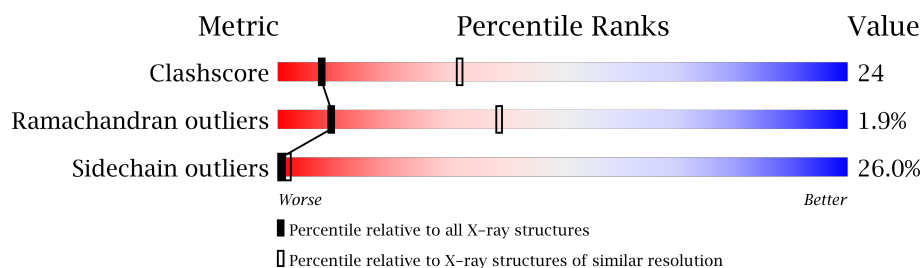
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)

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	395	
1	B	395	

2 Entry composition [i](#)

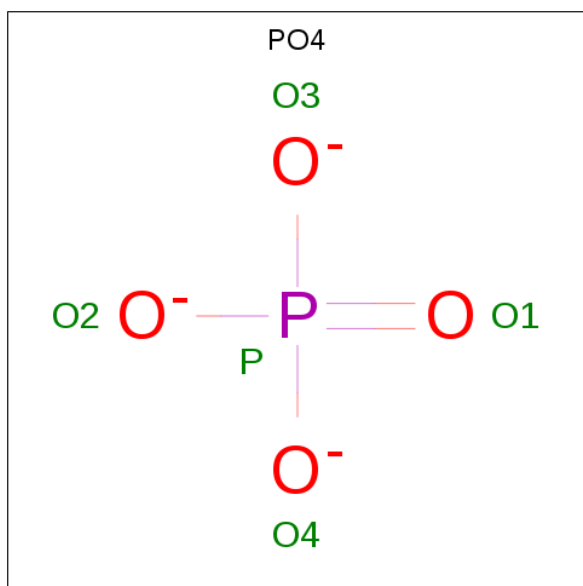
There are 2 unique types of molecules in this entry. The entry contains 6106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HEMOLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3048	1923	523	589	13			
1	B	391	Total	C	N	O	S	6	0	0
			3048	1923	523	589	13			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



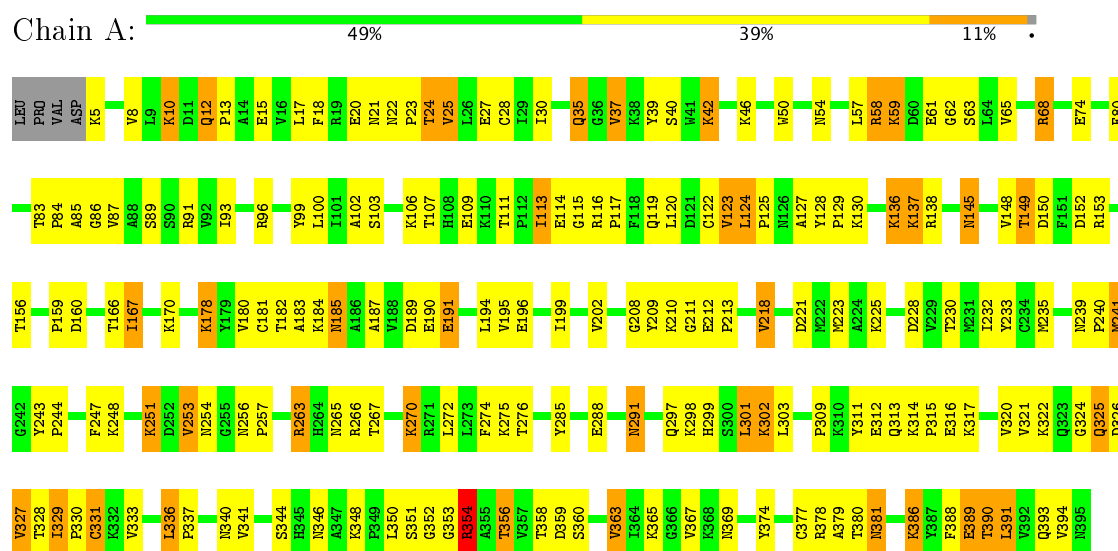
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

3 Residue-property plots

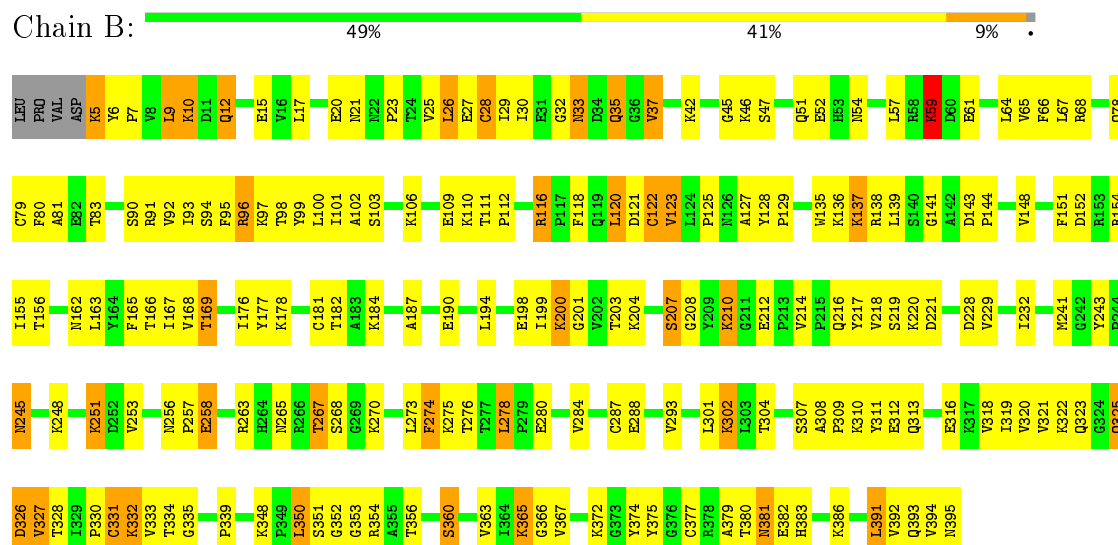
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: HEMOLIN



• Molecule 1: HEMOLIN



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	85.00 Å 90.30 Å 143.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	93.0 (20.00-3.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.857	Depositor
R, R_{free}	0.218 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6106	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: PO4

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	0.52	0/3119	0.68	0/4233
1	B	0.50	0/3119	0.68	0/4233
All	All	0.51	0/6238	0.68	0/8466

There are no bond length outliers.

There are no bond angle outliers.

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	3048	0	2992	157	0
1	B	3048	0	2992	140	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
All	All	6106	0	5984	290	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 (290) 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:B:96:ARG:HB3	1:B:96:ARG:HH11	1.28	0.95
1:B:122:CYS:SG	1:B:181:CYS:SG	2.64	0.92
1:A:309:PRO:HD3	1:A:381:ASN:HD21	1.31	0.91
1:B:122:CYS:HG	1:B:181:CYS:HG	0.89	0.88
1:A:291:ASN:HD22	1:A:291:ASN:H	1.21	0.87
1:A:288:GLU:HG3	1:A:298:LYS:HG2	1.56	0.87
1:A:145:ASN:HD22	1:A:145:ASN:H	1.27	0.82
1:A:316:GLU:O	1:A:390:THR:HB	1.79	0.81
1:A:180:VAL:HG22	1:A:196:GLU:HG2	1.61	0.80
1:B:318:VAL:HG23	1:B:391:LEU:HD23	1.63	0.80
1:B:331:CYS:SG	1:B:377:CYS:SG	2.55	0.80
1:A:122:CYS:SG	1:A:181:CYS:SG	2.52	0.79
1:A:331:CYS:SG	1:A:377:CYS:SG	2.65	0.79
1:A:322:LYS:H	1:A:325:GLN:NE2	1.80	0.78
1:A:18:PHE:HB2	1:A:24:THR:HG21	1.66	0.77
1:A:356:THR:HB	1:A:363:VAL:HG12	1.67	0.76
1:B:321:VAL:HG11	1:B:327:VAL:HG13	1.67	0.76
1:A:309:PRO:HD3	1:A:381:ASN:ND2	2.02	0.75
1:A:87:VAL:H	1:A:346:ASN:ND2	1.84	0.75
1:B:109:GLU:HG2	1:B:200:LYS:HG2	1.70	0.72
1:B:321:VAL:HG11	1:B:327:VAL:CG1	2.19	0.72
1:B:326:ASP:OD2	1:B:365:LYS:HG3	1.89	0.72
1:A:58:ARG:NH2	1:B:68:ARG:HD2	2.05	0.71
1:B:30:ILE:CD1	1:B:37:VAL:HG21	2.21	0.71
1:B:10:LYS:HB2	1:B:10:LYS:NZ	2.05	0.71
1:A:322:LYS:O	1:A:325:GLN:HG3	1.90	0.71
1:A:83:THR:HB	1:A:84:PRO:HD2	1.73	0.70
1:A:37:VAL:HB	1:A:83:THR:HG22	1.73	0.70
1:A:185:ASN:ND2	1:A:187:ALA:H	1.90	0.70
1:B:96:ARG:HB3	1:B:96:ARG:NH1	2.04	0.69
1:A:354:ARG:CZ	1:A:354:ARG:HB2	2.19	0.69
1:A:315:PRO:HB3	1:A:390:THR:HG22	1.75	0.69
1:A:50:TRP:CZ2	1:A:57:LEU:HD22	2.27	0.69
1:A:232:ILE:HD12	1:A:274:PHE:HE1	1.58	0.69
1:A:116:ARG:HG2	1:A:117:PRO:HD2	1.74	0.68
1:A:209:TYR:CE2	1:A:211:GLY:HA2	2.29	0.68
1:B:178:LYS:HD3	1:B:198:GLU:HG2	1.76	0.68
1:A:336:LEU:HD22	1:A:337:PRO:HA	1.75	0.68
1:B:5:LYS:HG3	1:B:32:GLY:HA2	1.74	0.68
1:B:267:THR:O	1:B:270:LYS:HD2	1.94	0.67
1:A:166:THR:HG21	1:A:241:MET:HG2	1.76	0.67
1:B:109:GLU:HG2	1:B:200:LYS:CG	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ASN:C	1:B:381:ASN:HD22	1.98	0.66
1:B:100:LEU:HA	1:B:127:ALA:HB2	1.78	0.66
1:B:6:TYR:CE2	1:B:393:GLN:HG2	2.31	0.66
1:A:145:ASN:N	1:A:145:ASN:HD22	1.94	0.66
1:A:99:TYR:CE1	1:A:127:ALA:HA	2.31	0.66
1:A:235:MET:HG2	1:A:270:LYS:HG2	1.78	0.65
1:B:42:LYS:HG2	1:B:47:SER:HA	1.79	0.65
1:A:321:VAL:HG23	1:A:394:VAL:HG23	1.78	0.65
1:A:42:LYS:HD2	1:A:80:PHE:CE2	2.32	0.65
1:B:316:GLU:OE1	1:B:319:ILE:HD11	1.97	0.65
1:A:58:ARG:CZ	1:B:68:ARG:HD2	2.27	0.64
1:B:30:ILE:HD12	1:B:37:VAL:HG21	1.80	0.64
1:A:232:ILE:HG23	1:A:301:LEU:HD12	1.80	0.64
1:B:30:ILE:HD11	1:B:81:ALA:HB1	1.79	0.64
1:A:331:CYS:HG	1:A:377:CYS:CB	2.11	0.64
1:B:12:GLN:NE2	1:B:90:SER:HB2	2.13	0.64
1:B:354:ARG:HB2	1:B:354:ARG:NH1	2.13	0.63
1:B:322:LYS:O	1:B:325:GLN:HG3	1.99	0.62
1:A:221:ASP:HA	1:A:301:LEU:HD23	1.82	0.62
1:B:28:CYS:SG	1:B:79:CYS:SG	2.68	0.62
1:B:381:ASN:ND2	1:B:383:HIS:H	1.99	0.61
1:A:100:LEU:HA	1:A:127:ALA:HB2	1.82	0.61
1:B:318:VAL:CG2	1:B:391:LEU:HD23	2.31	0.61
1:B:320:VAL:HA	1:B:393:GLN:O	2.01	0.61
1:A:35:GLN:HE21	1:A:35:GLN:HA	1.65	0.60
1:A:244:PRO:O	1:A:263:ARG:NH1	2.34	0.60
1:B:6:TYR:HB3	1:B:7:PRO:HD2	1.82	0.60
1:A:123:VAL:CG2	1:A:123:VAL:O	2.50	0.59
1:A:153:ARG:NH1	2:A:396:PO4:O1	2.36	0.59
1:A:87:VAL:H	1:A:346:ASN:HD22	1.49	0.59
1:B:321:VAL:O	1:B:394:VAL:HG23	2.02	0.59
1:B:321:VAL:HG23	1:B:394:VAL:HG23	1.85	0.58
1:A:183:ALA:HB3	1:A:194:LEU:HD21	1.86	0.58
1:A:185:ASN:HD21	1:A:187:ALA:HB3	1.68	0.58
1:A:21:ASN:ND2	1:A:68:ARG:HD3	2.19	0.58
1:B:42:LYS:HE3	1:B:80:PHE:CE2	2.39	0.58
1:A:113:ILE:HD12	1:A:113:ILE:H	1.68	0.57
1:A:128:TYR:CD1	1:A:129:PRO:HA	2.39	0.57
1:A:340:ASN:OD1	1:A:340:ASN:O	2.22	0.57
1:A:374:TYR:CE1	1:A:391:LEU:HG	2.40	0.57
1:B:123:VAL:O	1:B:194:LEU:HD13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:HB2	1:A:228:ASP:OD2	2.03	0.57
1:A:113:ILE:CD1	1:A:113:ILE:H	2.18	0.56
1:A:21:ASN:ND2	1:A:68:ARG:HH11	2.04	0.56
1:A:230:THR:HG21	1:A:303:LEU:HD11	1.87	0.56
1:B:6:TYR:HE2	1:B:393:GLN:HG2	1.69	0.56
1:A:113:ILE:HD12	1:A:113:ILE:N	2.20	0.56
1:B:78:GLN:HG2	1:B:80:PHE:CZ	2.41	0.56
1:A:42:LYS:HD2	1:A:80:PHE:HE2	1.69	0.55
1:A:185:ASN:HD22	1:A:185:ASN:C	2.10	0.55
1:B:135:TRP:CG	1:B:163:LEU:HD13	2.41	0.55
1:A:321:VAL:HB	1:A:325:GLN:HE21	1.71	0.55
1:B:253:VAL:O	1:B:253:VAL:HG12	2.07	0.55
1:B:210:LYS:O	1:B:293:VAL:HG11	2.07	0.55
1:B:166:THR:HG21	1:B:241:MET:HE2	1.89	0.55
1:A:324:GLY:H	1:A:367:VAL:HG12	1.71	0.55
1:B:335:GLY:HA3	1:B:339:PRO:HD3	1.89	0.55
1:B:109:GLU:CG	1:B:200:LYS:HG2	2.37	0.55
1:B:327:VAL:HG22	1:B:367:VAL:HG21	1.89	0.54
1:A:35:GLN:HE21	1:A:35:GLN:CA	2.20	0.54
1:A:58:ARG:HD2	1:A:65:VAL:CG2	2.37	0.54
1:A:21:ASN:HD22	1:A:68:ARG:HD3	1.73	0.54
1:B:94:SER:OG	1:B:96:ARG:HD3	2.06	0.54
1:A:178:LYS:HE2	1:A:196:GLU:OE2	2.07	0.54
1:A:183:ALA:CB	1:A:194:LEU:HD21	2.38	0.53
1:B:121:ASP:HA	1:B:162:ASN:OD1	2.08	0.53
1:A:248:LYS:O	1:A:251:LYS:HG3	2.08	0.53
1:B:20:GLU:O	1:B:21:ASN:HB2	2.08	0.53
1:A:247:PHE:HA	1:A:253:VAL:HG23	1.91	0.53
1:B:154:ARG:HA	1:B:241:MET:HE1	1.90	0.53
1:A:225:LYS:O	1:A:228:ASP:HB2	2.08	0.53
1:A:291:ASN:N	1:A:291:ASN:HD22	1.90	0.53
1:B:375:TYR:HD2	1:B:392:VAL:HG23	1.72	0.52
1:A:145:ASN:H	1:A:145:ASN:ND2	2.02	0.52
1:A:185:ASN:ND2	1:A:185:ASN:C	2.61	0.52
1:B:10:LYS:HB2	1:B:10:LYS:HZ3	1.74	0.52
1:A:213:PRO:HD3	1:A:291:ASN:ND2	2.24	0.52
1:B:327:VAL:HG22	1:B:367:VAL:CG2	2.39	0.52
1:A:137:LYS:HB3	1:A:149:THR:HG23	1.92	0.52
1:A:25:VAL:HG12	1:B:23:PRO:HG2	1.92	0.52
1:B:125:PRO:HD3	1:B:194:LEU:CD1	2.40	0.52
1:B:278:LEU:HB3	1:B:280:GLU:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PHE:CB	1:A:24:THR:HG21	2.37	0.52
1:A:21:ASN:HD21	1:A:68:ARG:HH11	1.55	0.52
1:A:123:VAL:HG23	1:A:123:VAL:O	2.08	0.52
1:A:330:PRO:O	1:A:331:CYS:HB2	2.10	0.52
1:A:315:PRO:CB	1:A:390:THR:HG22	2.40	0.52
1:B:351:SER:O	1:B:353:GLY:N	2.35	0.51
1:A:113:ILE:HD13	1:A:116:ARG:HB3	1.92	0.51
1:B:333:VAL:HG11	1:B:379:ALA:HB1	1.92	0.51
1:A:12:GLN:HG3	1:A:93:ILE:HD11	1.92	0.51
1:B:98:THR:HG23	1:B:187:ALA:HB2	1.92	0.51
1:A:333:VAL:HG11	1:A:379:ALA:CB	2.40	0.51
1:A:54:ASN:ND2	1:B:59:LYS:HB2	2.26	0.51
1:B:116:ARG:O	1:B:168:VAL:HG12	2.10	0.51
1:B:26:LEU:HD11	1:B:95:PHE:CD1	2.45	0.51
1:A:256:ASN:HB3	1:A:257:PRO:CD	2.41	0.51
1:B:311:TYR:HE1	1:B:386:LYS:HB3	1.74	0.51
1:A:232:ILE:HD12	1:A:274:PHE:CE1	2.44	0.50
1:B:166:THR:HG21	1:B:241:MET:CE	2.41	0.50
1:A:10:LYS:O	1:A:12:GLN:NE2	2.44	0.50
1:A:149:THR:HA	1:B:148:VAL:HG13	1.94	0.50
1:B:325:GLN:O	1:B:367:VAL:HG23	2.12	0.50
1:B:33:ASN:HD21	1:B:35:GLN:HB2	1.77	0.50
1:B:12:GLN:HE22	1:B:90:SER:HA	1.77	0.49
1:B:25:VAL:HG23	1:B:65:VAL:CG2	2.42	0.49
1:B:354:ARG:HD3	1:B:366:GLY:CA	2.42	0.49
1:A:232:ILE:HG12	1:A:301:LEU:CD1	2.41	0.49
1:A:315:PRO:HB3	1:A:390:THR:CG2	2.40	0.49
1:A:321:VAL:HG11	1:A:327:VAL:HB	1.94	0.49
1:A:285:TYR:N	1:A:301:LEU:O	2.41	0.49
1:A:311:TYR:CE2	1:A:388:PHE:HD2	2.31	0.49
1:A:136:LYS:HB3	1:A:148:VAL:HG13	1.94	0.49
1:A:96:ARG:HH11	1:A:96:ARG:HB3	1.77	0.49
1:B:102:ALA:HB2	1:B:125:PRO:HB3	1.93	0.49
1:A:119:GLN:HG3	1:A:119:GLN:O	2.11	0.49
1:A:22:ASN:ND2	1:A:23:PRO:HD2	2.28	0.49
1:B:54:ASN:OD1	1:B:67:LEU:HD12	2.13	0.49
1:A:329:ILE:HG22	1:A:390:THR:HG21	1.95	0.48
1:A:59:LYS:HG3	1:B:54:ASN:CG	2.34	0.48
1:A:301:LEU:CD2	1:A:302:LYS:N	2.76	0.48
1:A:351:SER:O	1:A:353:GLY:N	2.39	0.48
1:B:5:LYS:HG3	1:B:32:GLY:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ASN:HA	1:A:68:ARG:HG2	1.94	0.48
1:A:276:THR:O	1:A:276:THR:HG23	2.14	0.48
1:B:118:PHE:HB3	1:B:165:PHE:HB2	1.95	0.48
1:B:112:PRO:HD2	1:B:201:GLY:O	2.13	0.48
1:B:354:ARG:HD3	1:B:366:GLY:N	2.29	0.48
1:B:217:TYR:C	1:B:217:TYR:CD1	2.88	0.47
1:B:354:ARG:CB	1:B:354:ARG:HH11	2.27	0.47
1:A:389:GLU:O	1:A:389:GLU:HG2	2.13	0.47
1:A:58:ARG:HD2	1:A:65:VAL:HG21	1.95	0.47
1:B:120:LEU:HD22	1:B:165:PHE:CE1	2.49	0.47
1:B:116:ARG:HH22	1:B:207:SER:HB2	1.79	0.47
1:B:256:ASN:HB3	1:B:257:PRO:HD2	1.96	0.47
1:A:30:ILE:HG22	1:A:30:ILE:O	2.15	0.47
1:A:320:VAL:HA	1:A:393:GLN:O	2.14	0.47
1:B:51:GLN:HG2	1:B:52:GLU:N	2.29	0.47
1:B:33:ASN:ND2	1:B:35:GLN:HB2	2.29	0.47
1:B:381:ASN:C	1:B:381:ASN:ND2	2.64	0.47
1:B:120:LEU:HD22	1:B:165:PHE:HE1	1.80	0.47
1:B:35:GLN:HA	1:B:35:GLN:NE2	2.29	0.47
1:B:26:LEU:HD13	1:B:66:PHE:HE2	1.80	0.47
1:A:115:GLY:C	1:A:167:ILE:HG22	2.35	0.47
1:A:21:ASN:HD22	1:A:68:ARG:CD	2.28	0.47
1:B:128:TYR:CD1	1:B:129:PRO:HA	2.50	0.47
1:A:54:ASN:HD21	1:B:59:LYS:H	1.63	0.47
1:B:9:LEU:HD23	1:B:30:ILE:HG12	1.96	0.47
1:A:312:GLU:O	1:A:313:GLN:HG2	2.14	0.47
1:B:25:VAL:HG23	1:B:65:VAL:HG23	1.97	0.47
1:A:367:VAL:O	1:A:367:VAL:HG13	2.16	0.46
1:A:12:GLN:HB2	1:A:13:PRO:HD2	1.97	0.46
1:A:124:LEU:HD11	1:A:160:ASP:O	2.15	0.46
1:A:254:ASN:HB3	1:A:263:ARG:HG2	1.95	0.46
1:A:309:PRO:O	1:A:386:LYS:HE3	2.15	0.46
1:A:159:PRO:HG3	1:A:233:TYR:CE1	2.51	0.46
1:B:321:VAL:HG21	1:B:327:VAL:HG13	1.96	0.46
1:A:333:VAL:HG11	1:A:379:ALA:HB1	1.96	0.46
1:B:100:LEU:O	1:B:101:ILE:HD13	2.15	0.46
1:B:248:LYS:O	1:B:251:LYS:HG3	2.15	0.46
1:B:15:GLU:OE2	1:B:96:ARG:HG3	2.16	0.46
1:B:116:ARG:HH22	1:B:207:SER:CB	2.29	0.46
1:B:125:PRO:HD3	1:B:194:LEU:HD11	1.98	0.45
1:B:284:VAL:HG22	1:B:302:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:THR:OG1	1:A:150:ASP:N	2.49	0.45
1:B:154:ARG:HA	1:B:241:MET:CE	2.47	0.45
1:B:30:ILE:HG22	1:B:30:ILE:O	2.15	0.45
1:A:218:VAL:HG22	1:A:299:HIS:CD2	2.52	0.45
1:A:218:VAL:HG13	1:A:299:HIS:NE2	2.32	0.45
1:A:21:ASN:HD22	1:A:68:ARG:CG	2.30	0.45
1:A:42:LYS:CD	1:A:80:PHE:HE2	2.30	0.45
1:B:122:CYS:SG	1:B:194:LEU:HD12	2.57	0.45
1:A:256:ASN:HB3	1:A:257:PRO:HD2	1.99	0.45
1:B:258:GLU:N	1:B:258:GLU:OE1	2.44	0.45
1:A:230:THR:HG21	1:A:303:LEU:CD1	2.47	0.44
1:A:324:GLY:H	1:A:367:VAL:CG1	2.30	0.44
1:A:356:THR:CB	1:A:363:VAL:HG12	2.43	0.44
1:A:39:TYR:CD2	1:A:62:GLY:HA3	2.52	0.44
1:A:381:ASN:C	1:A:381:ASN:HD22	2.20	0.44
1:B:330:PRO:O	1:B:331:CYS:HB2	2.17	0.44
1:A:191:GLU:H	1:A:191:GLU:HG3	1.58	0.44
1:B:137:LYS:NZ	1:B:177:TYR:CD2	2.84	0.44
1:B:325:GLN:O	1:B:367:VAL:CG2	2.66	0.44
1:A:20:GLU:O	1:A:21:ASN:HB2	2.17	0.44
1:A:380:THR:HG22	1:A:381:ASN:N	2.33	0.43
1:B:248:LYS:HB2	1:B:253:VAL:HG21	1.99	0.43
1:B:322:LYS:O	1:B:323:GLN:C	2.56	0.43
1:A:311:TYR:CD1	1:A:333:VAL:HG22	2.54	0.43
1:B:122:CYS:HB2	1:B:181:CYS:SG	2.59	0.43
1:B:151:PHE:HB3	1:B:155:ILE:HD12	2.01	0.43
1:B:118:PHE:HE2	1:B:199:ILE:HD11	1.82	0.43
1:A:10:LYS:NZ	1:A:10:LYS:HB3	2.34	0.43
1:A:321:VAL:HA	1:A:325:GLN:NE2	2.34	0.43
1:B:221:ASP:OD1	1:B:302:LYS:N	2.50	0.43
1:A:267:THR:O	1:A:270:LYS:HB2	2.19	0.43
1:A:326:ASP:OD1	1:A:365:LYS:O	2.36	0.43
1:B:15:GLU:OE2	1:B:128:TYR:OH	2.31	0.43
1:B:328:THR:O	1:B:330:PRO:HD3	2.18	0.43
1:B:332:LYS:HG2	1:B:360:SER:HA	2.00	0.43
1:A:341:VAL:HA	1:A:378:ARG:O	2.19	0.43
1:A:86:GLY:HA3	1:A:346:ASN:HD21	1.84	0.43
1:B:217:TYR:CD1	1:B:218:VAL:N	2.87	0.43
1:B:27:GLU:HG2	1:B:29:ILE:CD1	2.49	0.43
1:B:374:TYR:CE2	1:B:391:LEU:HB2	2.53	0.43
1:A:322:LYS:N	1:A:325:GLN:NE2	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:VAL:HG22	1:A:329:ILE:HD13	2.00	0.43
1:A:21:ASN:ND2	1:A:68:ARG:NH1	2.66	0.43
1:B:167:ILE:HD12	1:B:169:THR:HG22	1.99	0.43
1:B:6:TYR:OH	1:B:320:VAL:HG21	2.19	0.43
1:B:394:VAL:HG22	1:B:395:ASN:H	1.84	0.43
1:A:363:VAL:CG1	1:A:363:VAL:O	2.66	0.42
1:A:21:ASN:HD22	1:A:68:ARG:HG2	1.83	0.42
1:B:308:ALA:HB1	1:B:309:PRO:HD2	2.00	0.42
1:B:99:TYR:CE1	1:B:127:ALA:HA	2.54	0.42
1:A:301:LEU:HD23	1:A:302:LYS:N	2.34	0.42
1:B:274:PHE:N	1:B:274:PHE:CD1	2.87	0.42
1:B:354:ARG:CB	1:B:354:ARG:NH1	2.80	0.42
1:A:248:LYS:HD2	1:A:285:TYR:OH	2.20	0.42
1:A:58:ARG:HG2	1:A:58:ARG:NH1	2.33	0.42
1:A:239:ASN:HA	1:A:240:PRO:HA	1.89	0.42
1:A:102:ALA:HB2	1:A:125:PRO:HB3	2.01	0.42
1:A:85:ALA:HB1	1:A:391:LEU:HD21	2.02	0.42
1:B:245:ASN:HB2	1:B:288:GLU:HG2	2.01	0.42
1:A:114:GLU:HG3	1:A:202:VAL:CG2	2.50	0.42
1:A:322:LYS:H	1:A:325:GLN:CD	2.23	0.41
1:B:99:TYR:O	1:B:127:ALA:HB1	2.20	0.41
1:B:122:CYS:CB	1:B:181:CYS:SG	3.08	0.41
1:A:328:THR:O	1:A:330:PRO:HD3	2.19	0.41
1:A:58:ARG:HB2	1:A:63:SER:HB2	2.02	0.41
1:A:291:ASN:N	1:A:291:ASN:ND2	2.61	0.41
1:B:30:ILE:HD11	1:B:81:ALA:CB	2.49	0.41
1:A:336:LEU:HA	1:A:337:PRO:C	2.41	0.41
1:B:321:VAL:O	1:B:394:VAL:CG2	2.68	0.41
1:B:335:GLY:CA	1:B:339:PRO:HD3	2.49	0.41
1:B:321:VAL:O	1:B:394:VAL:HA	2.20	0.41
1:A:336:LEU:HD22	1:A:337:PRO:CA	2.47	0.41
1:A:381:ASN:N	1:A:381:ASN:ND2	2.69	0.41
1:B:10:LYS:HB2	1:B:10:LYS:HZ2	1.85	0.41
1:B:333:VAL:HG11	1:B:379:ALA:CB	2.51	0.41
1:B:200:LYS:HG3	1:B:200:LYS:H	1.59	0.41
1:B:42:LYS:HD2	1:B:45:GLY:O	2.21	0.41
1:A:336:LEU:CD2	1:A:337:PRO:HA	2.46	0.41
1:B:125:PRO:HD3	1:B:194:LEU:HD13	2.03	0.41
1:B:351:SER:C	1:B:353:GLY:H	2.23	0.40
1:A:74:GLU:OE1	1:A:96:ARG:HD2	2.22	0.40
1:A:301:LEU:HD22	1:A:302:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASP:HA	1:B:144:PRO:HD2	1.87	0.40
1:B:354:ARG:HD3	1:B:366:GLY:H	1.87	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	389/395 (98%)	351 (90%)	31 (8%)	7 (2%)	10	40
1	B	389/395 (98%)	346 (89%)	35 (9%)	8 (2%)	8	36
All	All	778/790 (98%)	697 (90%)	66 (8%)	15 (2%)	9	39

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	208	GLY
1	B	59	LYS
1	B	141	GLY
1	B	208	GLY
1	B	350	LEU
1	A	28	CYS
1	A	350	LEU
1	B	28	CYS
1	A	331	CYS
1	B	331	CYS
1	A	354	ARG
1	B	152	ASP
1	A	352	GLY
1	B	352	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	333/340 (98%)	248 (74%)	85 (26%)	0	2
1	B	333/340 (98%)	245 (74%)	88 (26%)	0	1
All	All	666/680 (98%)	493 (74%)	173 (26%)	0	2

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	8	VAL
1	A	10	LYS
1	A	12	GLN
1	A	15	GLU
1	A	17	LEU
1	A	24	THR
1	A	25	VAL
1	A	27	GLU
1	A	35	GLN
1	A	37	VAL
1	A	40	SER
1	A	42	LYS
1	A	46	LYS
1	A	58	ARG
1	A	61	GLU
1	A	68	ARG
1	A	89	SER
1	A	91	ARG
1	A	103	SER
1	A	106	LYS
1	A	107	THR
1	A	109	GLU
1	A	111	THR
1	A	113	ILE
1	A	120	LEU
1	A	123	VAL

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Mol	Chain	Res	Type
1	A	124	LEU
1	A	130	LYS
1	A	136	LYS
1	A	137	LYS
1	A	138	ARG
1	A	145	ASN
1	A	149	THR
1	A	152	ASP
1	A	156	THR
1	A	167	ILE
1	A	170	LYS
1	A	178	LYS
1	A	182	THR
1	A	184	LYS
1	A	185	ASN
1	A	189	ASP
1	A	190	GLU
1	A	191	GLU
1	A	195	VAL
1	A	199	ILE
1	A	210	LYS
1	A	212	GLU
1	A	218	VAL
1	A	223	MET
1	A	241	MET
1	A	243	TYR
1	A	251	LYS
1	A	253	VAL
1	A	263	ARG
1	A	265	ASN
1	A	266	ARG
1	A	270	LYS
1	A	272	LEU
1	A	275	LYS
1	A	291	ASN
1	A	297	GLN
1	A	301	LEU
1	A	302	LYS
1	A	314	LYS
1	A	317	LYS
1	A	325	GLN
1	A	327	VAL

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Mol	Chain	Res	Type
1	A	329	ILE
1	A	336	LEU
1	A	344	SER
1	A	348	LYS
1	A	354	ARG
1	A	356	THR
1	A	358	THR
1	A	359	ASP
1	A	360	SER
1	A	363	VAL
1	A	369	ASN
1	A	381	ASN
1	A	386	LYS
1	A	389	GLU
1	A	390	THR
1	A	391	LEU
1	B	5	LYS
1	B	9	LEU
1	B	10	LYS
1	B	12	GLN
1	B	17	LEU
1	B	26	LEU
1	B	33	ASN
1	B	35	GLN
1	B	37	VAL
1	B	46	LYS
1	B	57	LEU
1	B	59	LYS
1	B	61	GLU
1	B	64	LEU
1	B	83	THR
1	B	91	ARG
1	B	92	VAL
1	B	93	ILE
1	B	96	ARG
1	B	97	LYS
1	B	103	SER
1	B	106	LYS
1	B	110	LYS
1	B	111	THR
1	B	116	ARG
1	B	120	LEU

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Mol	Chain	Res	Type
1	B	122	CYS
1	B	123	VAL
1	B	136	LYS
1	B	137	LYS
1	B	138	ARG
1	B	139	LEU
1	B	156	THR
1	B	169	THR
1	B	176	ILE
1	B	182	THR
1	B	184	LYS
1	B	190	GLU
1	B	200	LYS
1	B	203	THR
1	B	204	LYS
1	B	207	SER
1	B	210	LYS
1	B	212	GLU
1	B	214	VAL
1	B	216	GLN
1	B	219	SER
1	B	220	LYS
1	B	228	ASP
1	B	229	VAL
1	B	232	ILE
1	B	243	TYR
1	B	245	ASN
1	B	251	LYS
1	B	258	GLU
1	B	263	ARG
1	B	265	ASN
1	B	267	THR
1	B	268	SER
1	B	273	LEU
1	B	274	PHE
1	B	275	LYS
1	B	276	THR
1	B	278	LEU
1	B	287	CYS
1	B	301	LEU
1	B	302	LYS
1	B	304	THR

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Mol	Chain	Res	Type
1	B	307	SER
1	B	310	LYS
1	B	312	GLU
1	B	313	GLN
1	B	325	GLN
1	B	326	ASP
1	B	327	VAL
1	B	332	LYS
1	B	334	THR
1	B	348	LYS
1	B	350	LEU
1	B	356	THR
1	B	360	SER
1	B	363	VAL
1	B	365	LYS
1	B	372	LYS
1	B	380	THR
1	B	381	ASN
1	B	382	GLU
1	B	391	LEU

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

Mol	Chain	Res	Type
1	A	21	ASN
1	A	22	ASN
1	A	35	GLN
1	A	54	ASN
1	A	145	ASN
1	A	185	ASN
1	A	291	ASN
1	A	325	GLN
1	A	345	HIS
1	A	346	ASN
1	A	381	ASN
1	A	393	GLN
1	B	12	GLN
1	B	33	ASN
1	B	206	ASN
1	B	216	GLN
1	B	245	ASN
1	B	381	ASN

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Mol	Chain	Res	Type
1	B	393	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	PO4	A	396	-	4,4,4	0.52	0	6,6,6	0.76	0
2	PO4	B	396	-	4,4,4	0.71	0	6,6,6	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	396	-	-	0/0/0/0	0/0/0/0
2	PO4	B	396	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	396	PO4	1	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.