



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:56 PM EDT

PDB ID : 8CN9 / pdb_00008cn9
Title : Factor VII binding Fab of the bispecific antibody HMB-001 in complex with Factor VII
Authors : Schluckebier, G.; Johansson, E.
Deposited on : 2023-02-22
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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)	:	2.0
EDS	:	FAILED
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

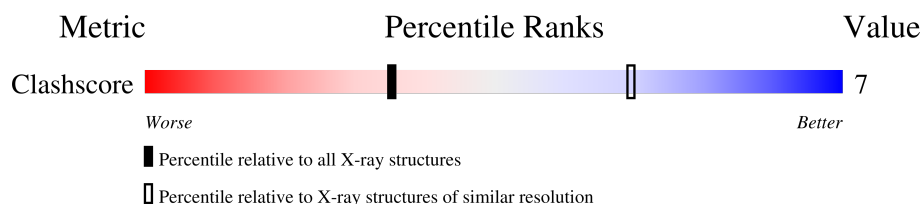
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1022 (3.44-3.36)

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	144.78Å 100.79Å 181.74Å 90.00° 101.22° 90.00°	Depositor
Resolution (Å)	48.50 – 3.40	Depositor
% Data completeness (in resolution range)	93.0 (48.50-3.40)	Depositor
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.303 , 0.356	Depositor
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.650	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29516	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1541e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

3 Model quality

3.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, CA, CS

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	0.08	0/1668	0.26	0/2267
1	F	0.09	0/1645	0.27	0/2237
1	K	0.09	0/1677	0.26	0/2279
1	P	0.08	0/1654	0.24	0/2246
2	B	0.09	0/1667	0.29	0/2277
2	G	0.09	0/1661	0.31	0/2269
2	L	0.08	0/1656	0.26	0/2263
2	Q	0.09	0/1661	0.28	0/2269
3	C	0.09	0/2024	0.24	0/2755
3	H	0.08	0/2024	0.22	0/2755
3	M	0.08	0/1987	0.25	0/2704
3	R	0.08	0/1987	0.23	0/2704
4	D	0.08	0/719	0.26	0/971
4	I	0.08	0/727	0.26	0/982
4	N	0.09	0/727	0.29	0/982
4	S	0.12	0/701	0.33	0/945
5	E	0.08	0/1637	0.26	0/2229
5	J	0.09	0/1583	0.26	0/2152
5	O	0.10	0/1402	0.29	0/1905
5	T	0.10	0/1347	0.29	0/1831
All	All	0.09	0/30154	0.26	0/41022

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

3.2 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	1630	0	1587	19	0
1	F	1607	0	1565	24	0
1	K	1639	0	1593	16	0
1	P	1617	0	1567	27	0
2	B	1627	0	1599	21	0
2	G	1621	0	1594	24	0
2	L	1616	0	1584	26	0
2	Q	1621	0	1594	23	0
3	C	1974	0	1950	39	0
3	H	1974	0	1951	24	0
3	M	1938	0	1912	36	0
3	R	1938	0	1913	39	0
4	D	706	0	639	13	0
4	I	714	0	644	4	0
4	N	714	0	644	15	0
4	S	689	0	620	14	0
5	E	1603	0	1543	22	0
5	J	1552	0	1511	32	0
5	O	1376	0	1337	25	0
5	T	1316	0	1270	22	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
6	H	2	0	0	0	0
6	K	1	0	0	0	0
6	M	2	0	0	0	0
6	R	2	0	0	0	0
7	D	11	0	8	0	0
7	I	11	0	9	0	0
7	S	11	0	8	0	0
8	P	1	0	0	0	0
All	All	29516	0	28642	428	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 7.

All (428) 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)
2:G:157:GLU:HG3	2:G:158:PRO:HA	1.57	0.84
1:K:113:PRO:HB3	1:K:139:PHE:HB3	1.67	0.76
2:B:210:LYS:HG3	2:B:211:PRO:HD3	1.66	0.76
5:J:134:VAL:HG23	5:J:141:LEU:HB2	1.72	0.71
1:K:187:GLU:HA	1:K:211:ARG:HH12	1.55	0.71
2:B:128:PRO:HB3	2:B:154:TYR:HB3	1.76	0.68
3:R:223:ARG:NH1	3:R:251:PRO:O	2.28	0.67
5:E:151:LEU:HA	5:E:193:ILE:HG22	1.77	0.66
5:O:20:LYS:HD2	5:O:60:THR:HG21	1.77	0.66
3:C:216:HIS:ND1	3:C:220:GLU:OE1	2.28	0.65
3:H:275:PHE:HB3	5:J:45:TRP:HB2	1.79	0.64
5:O:127:VAL:HG21	5:O:189:VAL:HG11	1.78	0.64
2:L:51:TYR:HE1	2:L:59:ASN:HB3	1.63	0.64
5:T:40:THR:HG23	5:T:43:GLY:HA3	1.79	0.64
2:L:128:PRO:HB3	2:L:154:TYR:HB3	1.79	0.64
5:J:36:VAL:HG22	5:J:75:VAL:HG22	1.78	0.63
3:M:273:LEU:HD11	3:M:357:TYR:HB2	1.81	0.63
1:A:42:GLU:OE1	1:A:45:ARG:NH2	2.31	0.63
2:Q:128:PRO:HB3	2:Q:154:TYR:HB3	1.81	0.63
5:J:6:THR:HG21	5:J:32:GLN:HB3	1.81	0.63
3:R:353:ARG:NH1	4:S:98:CYS:O	2.31	0.63
2:G:98:ARG:HG2	2:G:111:TYR:HB2	1.80	0.63
3:H:182:LEU:HD13	3:H:208:LEU:HD11	1.81	0.63
3:C:178:CYS:SG	3:C:344:SER:OG	2.56	0.62
3:C:184:ASN:HD21	3:C:187:TRP:HD1	1.47	0.62
5:O:113:ILE:HA	5:O:127:VAL:HG22	1.82	0.61
4:D:102:CYS:HA	4:D:112:CYS:HA	1.83	0.61
5:J:16:SER:O	5:J:107:ASN:ND2	2.34	0.61
5:O:113:ILE:HG23	5:O:125:VAL:HG13	1.82	0.61
2:L:53:GLN:NE2	2:L:57:SER:OG	2.34	0.61
5:J:6:THR:HG22	5:J:7:VAL:H	1.66	0.60
1:A:193:ALA:HB2	1:A:208:SER:HB3	1.83	0.60
3:M:182:LEU:HD22	3:M:208:LEU:HD11	1.82	0.60
1:F:15:PRO:HG3	1:F:106:ILE:HD11	1.83	0.60
1:K:90:ASN:ND2	1:K:93:SER:O	2.34	0.60
1:A:61:ARG:NH2	1:A:82:ASP:OD1	2.36	0.59
2:Q:103:TYR:HB3	3:R:184:ASN:HD22	1.67	0.59
3:R:255:THR:HG23	3:R:257:HIS:H	1.68	0.59
3:H:379:ARG:NH2	5:J:91:GLU:OE1	2.36	0.59
1:P:111:ALA:HB3	1:P:140:TYR:H	1.68	0.59
3:C:225:VAL:HG21	3:C:246:LEU:HD23	1.84	0.59
2:G:128:PRO:HB3	2:G:154:TYR:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:103:TYR:HB3	3:M:184:ASN:HD22	1.68	0.59
5:J:155:LEU:HD11	5:J:187:PHE:HB3	1.85	0.58
5:T:111:PRO:HB3	5:T:205:SER:HA	1.84	0.58
2:G:33:SER:HB3	2:G:98:ARG:HH21	1.69	0.58
3:R:228:VAL:HG22	3:R:246:LEU:HG	1.85	0.58
5:T:37:GLN:OE1	5:T:74:ARG:NH2	2.37	0.58
2:G:1:GLN:HG3	2:G:2:VAL:H	1.69	0.58
5:J:9:ALA:HA	5:J:27:PRO:HG3	1.85	0.57
1:P:21:LEU:HD12	1:P:73:LEU:HD23	1.84	0.57
3:R:229:ILE:HG21	3:R:390:LEU:HD13	1.86	0.57
4:S:102:CYS:SG	4:S:103:SER:N	2.76	0.57
1:A:6:GLN:HE21	1:A:102:THR:HG23	1.68	0.57
2:G:2:VAL:HG22	2:G:27:TYR:HB2	1.85	0.57
5:O:156:TYR:HA	5:O:167:THR:HA	1.86	0.57
1:K:14:SER:HA	1:K:107:LYS:HB2	1.87	0.57
3:C:161:LYS:NZ	3:C:217:ASP:OD2	2.37	0.57
1:F:46:LEU:HD21	1:F:49:LYS:HD3	1.86	0.57
5:J:155:LEU:HB3	5:J:168:ALA:HB3	1.87	0.57
3:R:277:ARG:HH21	5:T:43:GLY:H	1.52	0.56
3:C:223:ARG:HG3	3:C:252:VAL:HG12	1.87	0.56
1:P:79:GLU:HG3	1:P:80:PRO:HD2	1.87	0.56
1:P:108:ARG:HG2	1:P:109:THR:N	2.20	0.56
1:P:113:PRO:HB3	1:P:139:PHE:HB3	1.86	0.56
2:G:72:ARG:HE	2:G:74:THR:HG22	1.69	0.56
4:D:70:CYS:H	5:E:20:LYS:HE3	1.71	0.56
1:F:34:HIS:HD2	1:F:50:TYR:H	1.52	0.56
1:F:106:ILE:O	1:F:166:GLN:NE2	2.35	0.56
3:R:159:CYS:HB2	3:R:299:VAL:HG13	1.87	0.56
2:G:157:GLU:HG3	2:G:158:PRO:CA	2.31	0.56
1:P:106:ILE:O	1:P:166:GLN:NE2	2.38	0.56
3:R:300:LEU:HD21	3:R:337:LYS:HB3	1.88	0.56
4:N:102:CYS:SG	4:N:103:SER:N	2.80	0.55
2:G:164:ASN:ND2	2:G:202:THR:O	2.39	0.55
3:M:265:GLU:OE2	4:N:113:ARG:NH1	2.39	0.55
3:M:372:GLY:O	3:M:373:HIS:ND1	2.39	0.55
2:B:209:HIS:CD2	2:B:211:PRO:HD2	2.42	0.55
3:C:306:MET:HE1	5:E:76:PHE:HZ	1.71	0.55
3:M:327:MET:O	3:M:379:ARG:NH2	2.39	0.55
3:C:338:ASP:OD1	3:C:339:SER:N	2.37	0.55
3:M:172:VAL:HG12	3:M:177:LEU:HB2	1.87	0.55
2:B:73:ASP:OD1	2:B:73:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:151:LEU:HD12	5:E:153:TYR:HE1	1.71	0.55
3:R:242:ASP:OD2	3:R:363:SER:OG	2.24	0.54
3:C:186:ILE:HD13	3:C:251:PRO:HB3	1.89	0.54
3:H:202:ARG:O	3:H:224:ARG:NH1	2.39	0.54
3:M:277:ARG:HG2	3:M:303:PRO:HA	1.89	0.54
5:O:156:TYR:OH	5:O:204:ASP:OD2	2.25	0.54
4:D:61:CYS:SG	4:D:62:LYS:N	2.80	0.54
2:Q:32:ASP:HB2	3:R:251:PRO:HD3	1.88	0.54
4:S:73:LEU:HD12	4:S:75:ALA:H	1.73	0.54
2:B:154:TYR:HE2	2:B:157:GLU:HG2	1.72	0.54
1:K:47:LEU:HD23	1:K:48:ILE:HG12	1.89	0.54
2:L:209:HIS:CD2	2:L:211:PRO:HD2	2.42	0.54
2:Q:29:ILE:HD11	2:Q:74:THR:HA	1.88	0.54
4:D:73:LEU:HD23	4:D:73:LEU:H	1.73	0.53
5:J:11:ASN:ND2	5:J:26:GLU:OE1	2.39	0.53
5:J:16:SER:HB2	5:J:21:THR:HG23	1.90	0.53
5:E:26:GLU:HB2	5:E:27:PRO:HA	1.91	0.53
3:H:159:CYS:O	3:H:211:HIS:NE2	2.40	0.53
5:E:36:VAL:HG22	5:E:75:VAL:HG22	1.91	0.53
5:O:25:TRP:O	5:O:55:THR:OG1	2.27	0.53
1:P:47:LEU:HD23	1:P:58:ILE:HD12	1.91	0.53
2:Q:36:SER:HA	2:Q:51:TYR:HA	1.90	0.53
2:Q:105:ASN:HD22	4:S:117:GLY:HA3	1.74	0.53
2:L:18:LEU:HD12	2:L:118:VAL:HG11	1.90	0.53
3:H:172:VAL:HG22	3:H:177:LEU:HB2	1.91	0.53
3:H:229:ILE:HG21	3:H:390:LEU:HD13	1.91	0.53
2:Q:161:VAL:HG22	2:Q:207:VAL:HG22	1.91	0.53
3:R:172:VAL:HG21	3:R:198:ILE:HD11	1.90	0.53
3:C:300:LEU:HD21	3:C:337:LYS:HB3	1.91	0.53
5:J:193:ILE:HB	5:J:196:ARG:HD2	1.90	0.53
3:C:235:VAL:O	3:C:238:THR:OG1	2.27	0.52
4:S:68:TYR:OH	4:S:79:ARG:NH1	2.42	0.52
5:T:21:THR:N	5:T:60:THR:OG1	2.42	0.52
5:T:48:LYS:HD2	5:T:62:GLU:HG3	1.91	0.52
1:P:98:PHE:CG	2:Q:46:LEU:HD22	2.45	0.52
4:S:51:ALA:N	4:S:61:CYS:SG	2.72	0.52
3:M:245:LEU:HD13	3:M:387:LEU:HD22	1.91	0.52
1:K:33:LEU:HD21	1:K:88:CYS:HB2	1.91	0.52
5:T:35:THR:HG22	5:T:76:PHE:HB2	1.92	0.52
5:J:114:GLN:HG3	5:J:128:GLU:HB3	1.90	0.52
3:R:182:LEU:HD13	3:R:208:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:245:LEU:HD13	3:R:387:LEU:HD22	1.91	0.52
1:K:29:ILE:HD11	1:K:33:LEU:HD12	1.90	0.52
1:P:133:VAL:HG21	2:Q:133:LEU:HD13	1.91	0.52
5:E:152:ILE:HG12	5:E:194:PRO:HD3	1.92	0.51
1:F:80:PRO:HA	1:F:106:ILE:HD13	1.92	0.51
2:G:67:ARG:NH1	2:G:85:SER:O	2.43	0.51
2:L:92:ALA:HB3	2:L:94:TYR:HE1	1.74	0.51
3:C:208:LEU:HD22	3:C:258:VAL:HG13	1.93	0.51
5:J:113:ILE:HA	5:J:127:VAL:HG22	1.93	0.51
3:M:195:PHE:HB3	3:M:201:TRP:HH2	1.75	0.51
1:F:21:LEU:HD13	1:F:73:LEU:HD23	1.91	0.51
2:L:72:ARG:HA	2:L:79:PHE:HA	1.93	0.51
2:Q:204:THR:HG22	2:Q:219:ARG:HB3	1.91	0.51
1:K:125:LEU:HD22	1:K:183:LYS:HZ3	1.74	0.51
4:I:72:CYS:O	5:J:135:ARG:NH2	2.43	0.51
1:K:48:ILE:HD13	1:K:54:PRO:HA	1.93	0.51
5:O:12:LEU:HD22	5:O:97:SER:HB2	1.92	0.51
3:R:353:ARG:HD2	4:S:99:GLU:HA	1.92	0.51
5:T:108:LEU:HD11	5:T:193:ILE:HG13	1.91	0.51
1:A:125:LEU:HB3	1:A:183:LYS:HE3	1.93	0.51
5:T:38:ILE:HD12	5:T:59:LEU:HD13	1.93	0.51
3:C:166:TRP:CD2	3:C:261:LEU:HD13	2.46	0.50
1:P:21:LEU:HD22	1:P:102:THR:HG21	1.92	0.50
3:C:279:SER:HB2	3:C:348:HIS:NE2	2.26	0.50
2:G:130:VAL:HG21	2:G:207:VAL:HG21	1.92	0.50
2:G:164:ASN:HB3	2:G:167:ALA:HB3	1.93	0.50
3:M:217:ASP:OD1	3:M:217:ASP:N	2.43	0.50
4:S:120:LEU:HD21	4:S:124:GLY:HA2	1.92	0.50
1:K:107:LYS:HA	1:K:140:TYR:OH	2.11	0.50
3:C:256:ASP:OD1	4:D:133:TYR:OH	2.25	0.50
5:O:68:LYS:HG2	5:O:103:TYR:HE2	1.77	0.50
3:R:232:SER:HA	3:R:402:ARG:HG2	1.93	0.49
1:F:61:ARG:HH21	1:F:82:ASP:CG	2.19	0.49
5:T:145:ASP:O	5:T:147:PHE:N	2.42	0.49
1:P:88:CYS:O	1:P:99:GLY:N	2.45	0.49
3:C:208:LEU:HD12	3:C:252:VAL:HG11	1.94	0.49
5:J:127:VAL:HG21	5:J:189:VAL:HG21	1.93	0.49
3:C:160:PRO:HB2	3:C:163:GLU:HG3	1.94	0.49
3:C:167:GLN:OE1	3:C:282:SER:OG	2.27	0.49
1:F:13:LEU:HD12	1:F:17:GLU:HB3	1.95	0.49
2:G:2:VAL:HG11	2:G:98:ARG:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:100:PHE:CZ	5:O:102:PRO:HA	2.48	0.49
1:P:108:ARG:HD3	1:P:140:TYR:HB2	1.93	0.49
3:C:306:MET:HE1	5:E:76:PHE:CZ	2.47	0.49
3:H:255:THR:HG23	3:H:257:HIS:H	1.78	0.48
3:M:173:ASN:OD1	3:M:203:ASN:ND2	2.42	0.48
4:S:85:LYS:O	4:S:85:LYS:HD3	2.13	0.48
4:S:103:SER:HB2	4:S:113:ARG:HE	1.78	0.48
2:G:219:ARG:H	2:G:219:ARG:HD3	1.78	0.48
3:H:239:THR:HB	3:H:364:TRP:CD1	2.48	0.48
3:M:190:SER:OG	3:M:191:ALA:N	2.46	0.48
2:Q:98:ARG:HB3	2:Q:111:TYR:HB2	1.96	0.48
3:R:336:SER:OG	3:R:337:LYS:NZ	2.43	0.48
3:C:195:PHE:HE2	3:C:204:LEU:HD21	1.78	0.48
2:G:93:VAL:HG22	2:G:117:LEU:HD12	1.95	0.48
3:M:184:ASN:ND2	3:M:391:MET:HE3	2.28	0.48
5:E:39:SER:HB3	5:E:45:TRP:HA	1.94	0.48
3:H:279:SER:HB3	3:H:348:HIS:NE2	2.29	0.48
5:O:117:GLU:HB2	5:O:124:ASN:HB3	1.96	0.48
3:C:344:SER:HA	3:C:362:VAL:HG13	1.96	0.48
4:N:118:TYR:OH	4:N:135:CYS:O	2.30	0.48
1:F:37:GLN:HB2	1:F:47:LEU:HD11	1.96	0.48
5:T:143:LEU:HD23	5:T:143:LEU:H	1.78	0.48
2:G:154:TYR:OH	2:G:187:LEU:HD23	2.14	0.48
3:R:187:TRP:CZ3	3:R:247:ARG:HB2	2.49	0.48
4:S:102:CYS:HA	4:S:112:CYS:HA	1.95	0.48
2:G:36:SER:HA	2:G:51:TYR:HA	1.96	0.47
5:J:35:THR:HG23	5:J:50:PHE:HA	1.96	0.47
3:M:262:CYS:N	4:N:135:CYS:SG	2.87	0.47
3:R:153:ILE:N	3:R:343:ASP:OD2	2.47	0.47
3:M:338:ASP:OD1	3:M:339:SER:N	2.48	0.47
5:T:106:THR:O	5:T:196:ARG:NH1	2.48	0.47
5:J:136:ARG:HD3	5:J:141:LEU:HD21	1.96	0.47
5:J:143:LEU:O	5:J:146:VAL:N	2.47	0.47
2:L:37:TRP:HB3	2:L:49:ILE:HD11	1.96	0.47
4:N:69:ILE:HD12	5:O:20:LYS:HB3	1.95	0.47
5:O:6:THR:OG1	5:O:32:GLN:NE2	2.45	0.47
4:D:92:VAL:HG11	5:E:51:TYR:HE2	1.79	0.47
5:O:156:TYR:HB3	5:O:167:THR:HG22	1.97	0.47
3:R:338:ASP:OD1	3:R:339:SER:N	2.48	0.47
1:A:113:PRO:HB3	1:A:139:PHE:CB	2.45	0.47
1:K:94:PHE:HB2	4:N:130:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:343:ASP:OD1	3:R:343:ASP:N	2.33	0.47
3:M:287:LEU:HD11	3:M:294:ALA:HB2	1.97	0.47
3:R:165:PRO:HB2	3:R:259:VAL:HG12	1.97	0.47
2:B:18:LEU:HB2	2:B:86:VAL:HG11	1.96	0.46
2:B:18:LEU:HD11	2:B:118:VAL:HG11	1.97	0.46
4:D:103:SER:N	4:D:111:SER:O	2.43	0.46
5:E:28:LYS:HD3	5:E:55:THR:HG21	1.97	0.46
2:L:4:LEU:HD21	2:L:35:TRP:HZ3	1.79	0.46
1:F:134:CYS:HB2	1:F:148:TRP:CZ2	2.51	0.46
5:O:195:SER:HB3	5:O:196:ARG:HH21	1.80	0.46
5:O:110:GLN:HB3	5:O:203:THR:HG23	1.97	0.46
2:Q:51:TYR:CE1	2:Q:59:ASN:HB3	2.51	0.46
2:L:36:SER:HA	2:L:51:TYR:HA	1.97	0.46
1:F:161:GLU:HB3	1:F:175:LEU:HD21	1.98	0.46
2:L:103:TYR:HB3	3:M:184:ASN:ND2	2.30	0.46
4:N:69:ILE:HG23	5:O:20:LYS:HB2	1.97	0.46
1:P:118:PHE:HB2	1:P:133:VAL:HG23	1.98	0.46
5:T:32:GLN:NE2	5:T:34:TYR:OH	2.45	0.46
5:O:196:ARG:HB3	5:O:199:ASN:OD1	2.16	0.46
1:A:15:PRO:HG3	1:A:106:ILE:HD11	1.98	0.45
4:D:77:GLU:HB3	4:D:85:LYS:HD2	1.98	0.45
4:I:64:GLN:OE1	4:I:67:SER:OG	2.33	0.45
5:J:132:THR:OG1	5:J:141:LEU:O	2.33	0.45
2:B:6:GLU:OE2	2:B:115:GLY:N	2.49	0.45
3:C:234:TYR:HD2	3:C:402:ARG:HH12	1.64	0.45
1:P:70:ASP:OD1	1:P:70:ASP:N	2.49	0.45
3:C:166:TRP:CD1	3:C:261:LEU:HD22	2.52	0.45
1:P:138:ASN:HA	1:P:172:THR:HB	1.98	0.45
2:Q:53:GLN:HE21	2:Q:57:SER:HB2	1.82	0.45
3:R:190:SER:OG	3:R:191:ALA:N	2.50	0.45
3:C:172:VAL:HG12	3:C:177:LEU:HB2	1.99	0.45
5:E:86:THR:HA	5:E:89:ALA:HB2	1.99	0.45
1:F:142:ARG:HD3	1:F:163:VAL:HG11	1.99	0.45
2:G:37:TRP:CD2	2:G:81:LEU:HD23	2.52	0.45
1:K:170:ASP:OD1	1:K:170:ASP:N	2.43	0.45
1:K:187:GLU:N	1:K:211:ARG:HH22	2.15	0.45
3:M:229:ILE:HB	3:M:245:LEU:HB3	1.98	0.45
2:Q:16:GLN:HG3	2:Q:17:THR:H	1.82	0.45
2:B:161:VAL:HG22	2:B:207:VAL:HG22	1.98	0.45
3:C:229:ILE:HD13	3:C:390:LEU:HD13	1.98	0.45
5:O:38:ILE:HD11	5:O:59:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:209:HIS:ND1	2:Q:211:PRO:HD2	2.32	0.45
3:R:273:LEU:HD11	3:R:357:TYR:HB2	1.98	0.45
1:A:32:TYR:HB2	1:A:92:HIS:HB2	1.98	0.45
1:A:36:TYR:N	1:A:87:TYR:O	2.46	0.45
1:F:192:TYR:HB2	1:F:209:PHE:HE1	1.81	0.45
3:M:256:ASP:OD1	4:N:133:TYR:OH	2.28	0.45
1:P:33:LEU:HD22	1:P:71:PHE:CG	2.52	0.45
2:Q:156:PRO:C	2:Q:158:PRO:HD3	2.41	0.45
5:E:193:ILE:HG13	5:E:193:ILE:O	2.15	0.45
3:M:242:ASP:HB3	3:M:378:THR:HG21	1.99	0.45
3:M:208:LEU:HD22	3:M:258:VAL:HG22	1.98	0.45
3:M:227:GLN:HB2	3:M:247:ARG:HB3	1.98	0.45
3:R:232:SER:HB3	3:R:404:PRO:HA	1.97	0.45
1:A:28:GLY:HA3	4:D:113:ARG:HG2	1.98	0.45
1:F:110:VAL:HG23	1:F:140:TYR:O	2.16	0.45
3:H:161:LYS:HD3	3:H:211:HIS:CG	2.52	0.45
2:L:126:LYS:HA	2:L:126:LYS:HD3	1.71	0.45
2:Q:18:LEU:HD11	2:Q:118:VAL:HG11	1.98	0.45
2:G:126:LYS:HD2	2:G:184:LEU:HD21	1.99	0.44
3:H:169:LEU:HD11	3:H:176:GLN:HG2	1.98	0.44
3:M:161:LYS:NZ	3:M:217:ASP:OD2	2.50	0.44
1:A:133:VAL:HG22	1:A:178:THR:HB	2.00	0.44
3:C:300:LEU:HD11	3:C:337:LYS:HD3	1.99	0.44
2:Q:35:TRP:HB3	2:Q:79:PHE:CZ	2.53	0.44
5:T:17:THR:HG21	5:T:110:GLN:OE1	2.16	0.44
1:F:149:LYS:HE3	1:F:149:LYS:HB2	1.72	0.44
2:G:154:TYR:OH	2:G:177:ALA:HB2	2.17	0.44
1:P:187:GLU:HA	1:P:211:ARG:HH12	1.82	0.44
3:R:221:GLN:HE21	3:R:258:VAL:HG21	1.83	0.44
3:H:208:LEU:HD22	3:H:258:VAL:HG13	1.98	0.44
5:J:111:PRO:HG2	5:J:205:SER:OG	2.16	0.44
1:K:135:LEU:HD22	2:L:190:VAL:HG21	1.99	0.44
2:L:39:ARG:HH22	2:L:64:LEU:HD11	1.81	0.44
3:R:274:ALA:HB1	3:R:304:ARG:NH2	2.32	0.44
3:M:184:ASN:HD21	3:M:187:TRP:HD1	1.64	0.44
2:B:204:THR:HA	2:B:219:ARG:HA	1.99	0.44
5:J:45:TRP:CH2	5:J:74:ARG:HD3	2.52	0.44
4:N:106:THR:OG1	4:N:107:GLY:N	2.50	0.44
3:M:225:VAL:HG11	3:M:246:LEU:HD23	1.99	0.44
3:R:227:GLN:HB3	3:R:247:ARG:HB3	2.00	0.44
1:A:51:THR:HG21	1:A:71:PHE:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:232:SER:HA	3:C:402:ARG:HD2	2.00	0.44
5:E:172:THR:OG1	5:E:173:ASN:N	2.51	0.44
5:O:153:TYR:HE1	5:O:173:ASN:HA	1.82	0.44
3:C:168:VAL:HG21	3:C:188:VAL:HG21	2.00	0.43
2:L:54:TYR:HA	2:L:72:ARG:HH12	1.83	0.43
3:M:187:TRP:CD1	3:M:391:MET:HG3	2.53	0.43
3:M:208:LEU:HD23	3:M:209:GLY:N	2.33	0.43
2:B:6:GLU:HA	2:B:22:CYS:HA	2.01	0.43
1:F:94:PHE:O	1:F:96:LEU:N	2.51	0.43
2:L:49:ILE:HG22	2:L:64:LEU:HD12	2.00	0.43
3:M:187:TRP:CZ3	3:M:247:ARG:HB2	2.52	0.43
1:A:77:SER:O	1:A:77:SER:OG	2.30	0.43
3:H:159:CYS:HB2	3:H:299:VAL:HB	2.00	0.43
3:M:167:GLN:OE1	3:M:282:SER:OG	2.27	0.43
3:R:277:ARG:O	3:R:303:PRO:HA	2.18	0.43
2:B:164:ASN:HB3	2:B:167:ALA:HB3	1.99	0.43
3:C:225:VAL:HA	3:C:248:LEU:HA	2.01	0.43
5:J:32:GLN:HE22	5:J:77:SER:HB3	1.83	0.43
2:L:102:TYR:HD1	2:L:107:PHE:HB3	1.84	0.43
5:O:194:PRO:HA	5:O:200:ARG:CZ	2.48	0.43
1:P:89:GLN:HG3	1:P:98:PHE:CZ	2.54	0.43
3:R:214:SER:HB3	3:R:295:LEU:HD21	2.01	0.43
1:A:6:GLN:NE2	1:A:102:THR:HG23	2.33	0.43
1:A:6:GLN:OE1	1:A:99:GLY:HA3	2.19	0.43
1:F:120:PRO:HD3	1:F:132:VAL:HG22	2.01	0.43
5:J:157:TYR:HD2	5:J:165:LYS:HB3	1.83	0.43
1:F:105:GLU:OE1	1:F:173:TYR:OH	2.29	0.43
5:J:188:SER:HB2	5:J:207:VAL:HG22	2.00	0.43
5:T:39:SER:HB3	5:T:45:TRP:HD1	1.83	0.43
5:J:154:THR:HG23	5:J:190:GLN:HB3	2.01	0.43
3:C:217:ASP:OD1	3:C:217:ASP:N	2.43	0.43
3:R:272:THR:HG21	4:S:95:ASN:HB2	2.01	0.43
5:T:19:PHE:H	5:T:106:THR:HG23	1.83	0.43
2:B:51:TYR:CE1	2:B:59:ASN:HB3	2.54	0.43
2:L:93:VAL:HG22	2:L:117:LEU:HD13	2.00	0.43
2:B:34:ALA:HB1	2:B:51:TYR:CD2	2.54	0.42
5:E:144:ARG:HH11	5:E:151:LEU:HG	1.83	0.42
2:L:11:LEU:HD12	2:L:156:PRO:HG3	1.99	0.42
2:L:53:GLN:HG2	2:L:54:TYR:N	2.34	0.42
3:R:316:LYS:HE3	3:R:316:LYS:HB3	1.83	0.42
2:B:98:ARG:HD2	2:B:111:TYR:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:32:ASP:HB2	3:M:251:PRO:HD3	2.01	0.42
3:M:386:TRP:CD1	3:M:405:PHE:HA	2.55	0.42
4:D:70:CYS:N	5:E:20:LYS:HE3	2.34	0.42
3:H:263:LEU:HD12	3:H:264:PRO:HD2	2.01	0.42
3:H:338:ASP:OD1	3:H:339:SER:N	2.53	0.42
4:N:48:ASP:HB3	4:N:63:ASP:OD2	2.19	0.42
1:P:158:ASN:OD1	1:P:158:ASN:N	2.52	0.42
3:C:184:ASN:HD21	3:C:187:TRP:CD1	2.31	0.42
5:T:15:LYS:HE3	5:T:15:LYS:HB2	1.91	0.42
3:H:245:LEU:HD13	3:H:387:LEU:HD22	2.01	0.42
1:P:187:GLU:HA	1:P:211:ARG:NH1	2.35	0.42
3:C:187:TRP:CZ3	3:C:247:ARG:HB2	2.54	0.42
4:D:118:TYR:HD1	4:D:129:PRO:HA	1.84	0.42
3:H:306:MET:SD	5:J:74:ARG:NH2	2.92	0.42
2:L:52:ILE:HA	2:L:58:THR:HG22	2.01	0.42
3:M:193:HIS:ND1	3:M:242:ASP:OD2	2.52	0.42
1:F:192:TYR:HB2	1:F:209:PHE:CE1	2.55	0.42
2:G:125:THR:HG23	2:G:156:PRO:HD2	2.01	0.42
5:E:67:VAL:O	5:E:102:PRO:HG2	2.19	0.42
2:Q:35:TRP:HB2	2:Q:52:ILE:HG23	2.02	0.42
2:B:154:TYR:HB2	2:B:209:HIS:CE1	2.55	0.41
4:N:62:LYS:HD3	4:N:62:LYS:HA	1.87	0.41
4:N:138:ILE:HG22	4:N:140:ILE:HG12	2.02	0.41
5:E:111:PRO:HG2	5:E:205:SER:HB3	2.01	0.41
5:O:40:THR:HG22	5:O:71:TYR:HE1	1.85	0.41
1:P:95:PRO:HG3	2:Q:62:PRO:HD2	2.02	0.41
1:P:108:ARG:HG2	1:P:109:THR:H	1.84	0.41
2:Q:51:TYR:HE1	2:Q:59:ASN:HB3	1.85	0.41
5:T:101:THR:HG21	5:T:104:LEU:HB2	2.02	0.41
3:H:265:GLU:OE2	4:I:113:ARG:NH2	2.52	0.41
5:J:136:ARG:HH11	5:J:141:LEU:HD21	1.85	0.41
4:N:120:LEU:HA	4:N:127:CYS:HA	2.03	0.41
1:P:115:VAL:HA	1:P:135:LEU:O	2.21	0.41
3:R:201:TRP:HE1	3:R:228:VAL:HG21	1.85	0.41
3:C:242:ASP:OD2	3:C:363:SER:OG	2.27	0.41
4:D:96:GLY:O	4:D:110:ARG:NE	2.52	0.41
5:E:16:SER:HA	5:E:20:LYS:O	2.20	0.41
3:M:329:CYS:HA	3:M:376:VAL:HA	2.02	0.41
5:O:136:ARG:HB2	5:O:141:LEU:HD21	2.01	0.41
2:B:54:TYR:O	2:B:55:SER:OG	2.33	0.41
3:C:182:LEU:HD13	3:C:208:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:LYS:HE3	1:F:189:HIS:CE1	2.55	0.41
1:K:120:PRO:HD3	1:K:132:VAL:HG22	2.03	0.41
5:T:110:GLN:O	5:T:111:PRO:C	2.62	0.41
5:T:111:PRO:HD3	5:T:203:THR:CG2	2.50	0.41
2:B:150:LEU:HD21	2:B:152:LYS:HD3	2.01	0.41
3:C:348:HIS:O	3:C:359:THR:HG22	2.20	0.41
4:D:69:ILE:HG22	5:E:20:LYS:HD2	2.03	0.41
1:F:207:LYS:HB3	1:F:207:LYS:HE2	1.87	0.41
1:P:39:LYS:HG2	1:P:84:ALA:HB2	2.01	0.41
1:P:50:TYR:CE2	3:R:392:ARG:HG3	2.56	0.41
2:Q:24:VAL:HG11	2:Q:35:TRP:CH2	2.56	0.41
3:R:185:THR:HG22	3:R:254:LEU:HD21	2.02	0.41
1:A:4:LEU:HD21	1:A:88:CYS:SG	2.60	0.41
1:A:34:HIS:HD2	1:A:50:TYR:H	1.67	0.41
1:F:78:LEU:HD21	1:F:104:LEU:HD21	2.02	0.41
3:M:173:ASN:HA	3:M:203:ASN:ND2	2.36	0.41
4:S:73:LEU:HB2	4:S:74:PRO:HD2	2.02	0.41
3:H:254:LEU:HD22	3:H:260:PRO:HD3	2.02	0.41
3:H:277:ARG:HE	3:H:303:PRO:HB3	1.86	0.41
3:M:354:GLY:O	4:N:137:LYS:NZ	2.53	0.41
3:R:357:TYR:OH	4:S:100:GLN:HG3	2.21	0.41
1:A:11:LEU:HD21	1:A:13:LEU:HD12	2.03	0.41
2:B:195:SER:HA	2:B:198:LEU:HD13	2.02	0.41
3:C:338:ASP:HB3	3:C:369:ALA:H	1.85	0.41
2:G:11:LEU:HD12	2:G:156:PRO:HG3	2.02	0.41
3:H:217:ASP:OD1	3:H:217:ASP:N	2.43	0.41
1:K:182:SER:C	1:K:184:ALA:H	2.28	0.41
2:L:41:PRO:HD2	2:L:45:GLY:O	2.21	0.41
2:Q:72:ARG:HA	2:Q:79:PHE:HA	2.02	0.41
3:R:389:LYS:HG2	3:R:390:LEU:HG	2.02	0.41
5:E:33:VAL:HG23	5:E:78:TYR:HB2	2.03	0.41
1:F:38:GLN:CD	2:G:40:GLN:HE22	2.28	0.41
2:G:41:PRO:HA	2:G:92:ALA:HA	2.03	0.41
5:J:157:TYR:CE2	5:J:166:LYS:HG3	2.56	0.41
1:F:39:LYS:HG3	1:F:40:PRO:HD2	2.03	0.40
5:J:37:GLN:OE1	5:J:47:SER:OG	2.33	0.40
2:L:52:ILE:HD11	2:L:72:ARG:HD3	2.03	0.40
2:L:53:GLN:HG2	2:L:54:TYR:H	1.86	0.40
2:B:91:THR:HG23	2:B:119:THR:HA	2.03	0.40
3:C:261:LEU:HD12	3:C:261:LEU:HA	1.91	0.40
3:C:332:TYR:CE1	3:C:337:LYS:HD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:230:ILE:HD12	3:H:400:LEU:HD11	2.04	0.40
1:P:77:SER:O	1:P:77:SER:OG	2.37	0.40
1:P:139:PHE:HZ	1:P:175:LEU:HB2	1.86	0.40
3:H:229:ILE:HB	3:H:245:LEU:HB3	2.02	0.40
4:I:62:LYS:HD3	4:I:69:ILE:HD11	2.03	0.40
4:N:82:GLU:CD	4:N:82:GLU:H	2.29	0.40
5:O:150:ASP:O	5:O:193:ILE:HG22	2.21	0.40
5:T:111:PRO:HG3	5:T:204:ASP:O	2.21	0.40
1:A:12:SER:HA	1:A:105:GLU:O	2.21	0.40
2:B:53:GLN:HG2	2:B:54:TYR:O	2.22	0.40
3:C:325:GLU:H	3:C:325:GLU:CD	2.29	0.40
5:E:155:LEU:O	5:E:168:ALA:N	2.46	0.40
5:J:178:ASP:OD1	5:J:178:ASP:N	2.50	0.40
5:T:111:PRO:HD3	5:T:203:THR:HG23	2.04	0.40
5:O:153:TYR:H	5:O:153:TYR:HD1	1.70	0.40
3:R:366:GLN:HG2	3:R:373:HIS:CD2	2.57	0.40
3:R:383:TYR:O	3:R:387:LEU:N	2.43	0.40

There are no symmetry-related clashes.

3.3 Torsion angles [i](#)

3.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

3.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

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.

3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

4.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

4.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

4.4 Ligands

EDS failed to run properly - this section is therefore empty.

4.5 Other polymers

EDS failed to run properly - this section is therefore empty.