



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:25 AM UTC

PDB ID : 2Y07 / pdb_00002y07
Title : CRYSTAL STRUCTURE ANALYSIS OF THE ANTI-(4-HYDROXY-3-NITROPHENYL) - ACETYL MURINE GERMLINE MONOCLONAL ANTIBODY BBE6.12H3 FAB FRAGMENT IN COMPLEX WITH A PHAGE DISPLAY DERIVED DODECAPEPTIDE PPYPAWHAPGNI
Authors : Khan, T.; Salunke, D.M.
Deposited on : 2010-11-30
Resolution : 2.40 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

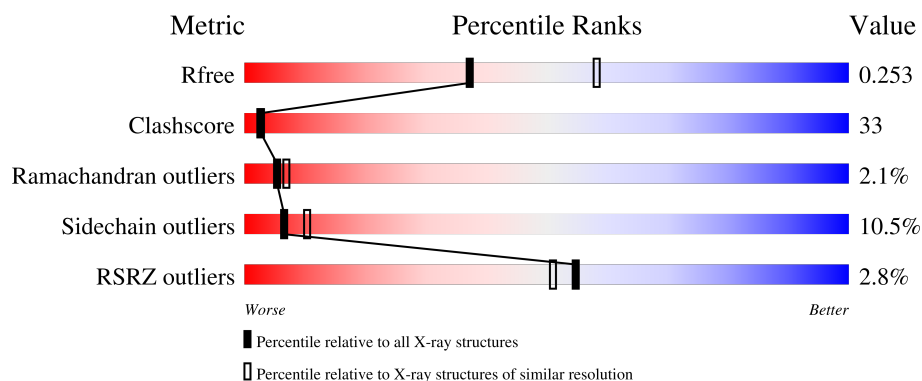
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	H	220	4% 50% 35% 10% ..
2	L	211	% 54% 40% 5% .
3	P	12	8% 8% 8% 17% 17% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3405 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 ANTI-NP MURINE GERMLINE MONOCLONAL ANTI-BODY BBE6.12H3, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	215	Total	C	N	O	S	0	0	0
			1619	1032	263	317	7			

- Molecule 2 is a protein called ANTI-NP MURINE GERMLINE MONOCLONAL ANTI-BODY BBE6.12H3, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1585	989	264	326	6			

- Molecule 3 is a protein called PHAGE DISPLAY DERIVED ANTIGEN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	6	Total	C	N	O	0	0	0
			52	38	7	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	81	Total	O	0	0
			81	81		
4	L	68	Total	O	0	0
			68	68		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	54.36Å 60.83Å 111.72Å 90.00° 94.79° 90.00°	Depositor
Resolution (Å)	23.62 – 2.40 23.62 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.6 (23.62-2.40) 91.6 (23.62-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.59 (at 2.41Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.257 0.238 , 0.253	Depositor DCC
R_{free} test set	1395 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3405	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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.

5 Model quality

5.1 Standard geometry

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	H	0.54	0/1668	1.16	14/2283 (0.6%)
2	L	1.11	20/1623 (1.2%)	1.16	14/2223 (0.6%)
3	P	1.00	0/57	2.38	3/80 (3.8%)
All	All	0.87	20/3348 (0.6%)	1.20	31/4586 (0.7%)

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
2	L	0	3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	159	THR	C-O	-13.83	1.11	1.24
2	L	143	TYR	C-O	-12.72	1.07	1.24
2	L	159	THR	CB-CG2	-10.71	1.17	1.52
2	L	144	PRO	CG-CD	-9.66	1.25	1.51
2	L	157	PRO	C-O	-8.70	1.13	1.23
2	L	144	PRO	CB-CG	-8.10	1.19	1.51
2	L	143	TYR	CZ-OH	-7.90	1.21	1.38
2	L	143	TYR	CD1-CE1	-7.83	1.15	1.38
2	L	156	THR	C-N	-7.57	1.24	1.33
2	L	144	PRO	N-CA	-7.57	1.34	1.47
2	L	158	VAL	C-N	-7.34	1.23	1.33
2	L	144	PRO	C-O	-7.25	1.08	1.23
2	L	157	PRO	CG-CD	-7.17	1.26	1.50
2	L	157	PRO	N-CA	-7.04	1.38	1.47
2	L	144	PRO	N-CD	-6.69	1.38	1.47
2	L	143	TYR	CE2-CZ	-6.57	1.22	1.38
2	L	144	PRO	CA-CB	-6.12	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	143	TYR	C-N	-5.62	1.23	1.34
2	L	143	TYR	CD2-CE2	-5.08	1.23	1.38
2	L	159	THR	CB-OG1	-5.04	1.35	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	159	THR	CB-CA-C	12.15	133.76	117.23
1	H	155	GLU	C-N-CD	-11.93	94.35	120.60
3	P	1	PRO	CA-C-N	11.27	133.92	119.84
3	P	1	PRO	C-N-CA	11.27	133.92	119.84
1	H	56	GLY	N-CA-C	-10.71	100.53	115.32
1	H	169	GLY	N-CA-C	-10.39	102.71	115.08
2	L	109	LEU	N-CA-C	-7.71	98.47	109.96
1	H	150	LYS	N-CA-C	7.64	121.88	109.59
1	H	219	PRO	N-CA-C	7.57	122.70	112.48
2	L	143	TYR	C-N-CD	-7.48	104.14	120.60
2	L	184	THR	N-CA-C	-7.41	99.51	110.48
2	L	143	TYR	O-C-N	7.23	129.64	121.32
2	L	33	ASN	N-CA-C	-7.22	104.47	113.28
1	H	107	PHE	N-CA-C	7.21	121.91	113.18
1	H	109	TYR	N-CA-C	7.08	121.22	109.46
1	H	61	ASN	N-CA-C	-6.92	99.58	109.96
2	L	144	PRO	N-CA-CB	-6.29	95.68	102.60
2	L	141	ASP	N-CA-C	6.00	119.70	111.54
2	L	26	THR	N-CA-C	-5.85	104.98	111.36
1	H	108	ASP	N-CA-C	5.81	123.18	110.80
3	P	2	PRO	N-CA-C	5.73	124.28	112.47
2	L	3	VAL	N-CA-C	-5.65	99.74	107.99
2	L	204	THR	N-CA-C	5.62	118.39	109.24
2	L	46	PHE	N-CA-C	5.57	117.38	108.41
2	L	160	GLN	N-CA-C	-5.55	100.28	108.99
1	H	111	GLY	N-CA-C	-5.51	103.98	112.85
1	H	206	HIS	CA-C-N	5.45	126.65	119.84
1	H	206	HIS	C-N-CA	5.45	126.65	119.84
1	H	13	LYS	CA-C-N	5.40	125.71	119.93
1	H	13	LYS	C-N-CA	5.40	125.71	119.93
2	L	144	PRO	CB-CG-CD	5.39	117.80	105.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	143	TYR	Peptide
2	L	158	VAL	Peptide
2	L	159	THR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1619	0	1565	124	0
2	L	1585	0	1515	87	0
3	P	52	0	47	25	0
4	H	81	0	0	8	0
4	L	68	0	0	5	0
All	All	3405	0	3127	213	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 33.

All (213) 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:H:155:GLU:CG	1:H:156:PRO:HB3	1.85	1.05
1:H:155:GLU:HG3	1:H:156:PRO:HB3	1.43	1.01
1:H:106:TYR:HB3	2:L:51:GLY:HA3	1.39	0.99
1:H:12:VAL:HG21	1:H:18:VAL:CG1	1.93	0.98
1:H:155:GLU:HG3	1:H:156:PRO:CA	1.94	0.97
1:H:93:VAL:HG22	1:H:115:THR:HG22	1.47	0.97
1:H:155:GLU:HG3	1:H:156:PRO:CB	1.93	0.97
1:H:71:THR:HG22	1:H:80:TYR:HB2	1.45	0.94
3:P:3:TYR:CD1	3:P:4:PRO:HD3	2.02	0.94
2:L:93:TRP:CD1	3:P:1:PRO:H3	1.86	0.94
1:H:155:GLU:HG3	1:H:156:PRO:HA	1.53	0.89
1:H:155:GLU:HG2	1:H:156:PRO:HB3	1.56	0.87
2:L:143:TYR:HA	2:L:144:PRO:O	1.74	0.86
1:H:142:MET:HE2	1:H:189:THR:HG22	1.59	0.85
1:H:126:PRO:HB3	1:H:152:TYR:HB3	1.60	0.84
2:L:32:SER:HB2	3:P:1:PRO:HG3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:63:ARG:CZ	2:L:80:GLN:HG3	2.08	0.82
2:L:158:VAL:HA	2:L:159:THR:HG22	1.61	0.82
1:H:191:PRO:O	1:H:194:PRO:HD2	1.81	0.81
1:H:98:ARG:HD2	1:H:108:ASP:OD2	1.80	0.81
2:L:123:PRO:HB2	2:L:128:LEU:HD11	1.63	0.80
1:H:12:VAL:HG21	1:H:18:VAL:HG12	1.64	0.80
2:L:143:TYR:HA	2:L:144:PRO:C	2.05	0.78
2:L:158:VAL:HG13	2:L:158:VAL:O	1.81	0.78
1:H:162:ASN:HB3	1:H:165:SER:HB2	1.66	0.78
1:H:12:VAL:HG21	1:H:18:VAL:HG11	1.65	0.78
1:H:100:ASP:O	1:H:105:SER:HA	1.85	0.77
2:L:197:GLN:HG3	2:L:206:GLU:HB2	1.68	0.76
1:H:38:LYS:HE2	1:H:40:ARG:HD2	1.68	0.76
2:L:39:GLN:HB2	2:L:49:LEU:HD11	1.66	0.76
1:H:142:MET:CE	1:H:189:THR:HG22	2.16	0.75
1:H:184:LEU:HD12	1:H:185:SER:N	2.02	0.74
2:L:172:ASN:O	2:L:173:ASN:HB2	1.89	0.73
1:H:142:MET:HB2	4:H:2060:HOH:O	1.88	0.73
1:H:104:GLY:O	1:H:105:SER:HB2	1.87	0.72
2:L:158:VAL:O	2:L:158:VAL:CG1	2.38	0.72
1:H:106:TYR:HB2	4:H:2048:HOH:O	1.89	0.72
1:H:30:THR:HB	1:H:54:ASN:OD1	1.89	0.71
1:H:33:TRP:CE3	1:H:50:ARG:HD2	2.25	0.70
2:L:95:SER:O	2:L:96:ASN:HB3	1.92	0.69
2:L:50:ILE:HD13	2:L:56:ARG:HA	1.73	0.69
1:H:50:ARG:HH12	3:P:4:PRO:HG3	1.55	0.69
2:L:32:SER:HB2	3:P:1:PRO:CG	2.23	0.69
1:H:115:THR:HG23	4:H:2006:HOH:O	1.91	0.69
1:H:83:LEU:HB3	1:H:86:LEU:HD11	1.76	0.68
2:L:63:ARG:NE	2:L:80:GLN:HG3	2.09	0.68
1:H:166:LEU:HG	1:H:188:VAL:HG21	1.76	0.68
1:H:157:VAL:HG12	1:H:206:HIS:CD2	2.29	0.67
2:L:32:SER:O	3:P:1:PRO:HG3	1.95	0.67
2:L:20:LEU:HB3	4:L:2009:HOH:O	1.93	0.66
1:H:152:TYR:CE2	1:H:157:VAL:HG13	2.29	0.66
2:L:2:ALA:O	2:L:99:VAL:HG11	1.96	0.65
1:H:100:ASP:OD1	1:H:106:TYR:CD1	2.49	0.65
1:H:163:SER:H	1:H:203:ASN:HD21	1.45	0.65
1:H:106:TYR:CD1	1:H:106:TYR:N	2.65	0.64
2:L:128:LEU:HD21	2:L:188:TRP:CD1	2.34	0.62
1:H:106:TYR:CE2	2:L:57:ALA:HA	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:180:ASP:HA	4:H:2072:HOH:O	1.99	0.62
1:H:131:LEU:HB2	1:H:146:GLY:CA	2.32	0.60
1:H:168:SER:C	1:H:170:VAL:H	2.10	0.59
1:H:178:GLN:OE1	2:L:163:GLU:HG3	2.02	0.59
2:L:6:GLN:NE2	2:L:90:CYS:H	2.00	0.59
1:H:50:ARG:HG2	1:H:51:ILE:N	2.17	0.59
1:H:193:SER:N	1:H:194:PRO:HD2	2.18	0.59
2:L:95:SER:HA	3:P:1:PRO:H2	1.67	0.59
1:H:18:VAL:HG22	1:H:86:LEU:HD21	1.84	0.59
2:L:151:TRP:HD1	2:L:162:MET:HE2	1.67	0.59
1:H:199:THR:CG2	1:H:200:VAL:N	2.66	0.58
1:H:51:ILE:HD13	1:H:72:VAL:HG13	1.85	0.58
1:H:155:GLU:CG	1:H:156:PRO:CB	2.62	0.58
2:L:6:GLN:HE22	2:L:90:CYS:H	1.51	0.58
1:H:196:PRO:O	1:H:197:SER:C	2.46	0.58
1:H:126:PRO:CB	1:H:152:TYR:HB3	2.33	0.57
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.86	0.57
2:L:108:VAL:O	2:L:109:LEU:C	2.45	0.57
1:H:37:VAL:HG11	1:H:45:LEU:HD22	1.86	0.57
1:H:76:SER:OG	1:H:78:THR:HG23	2.04	0.57
3:P:4:PRO:HD2	3:P:6:TRP:CD1	2.40	0.56
2:L:68:LEU:HD23	2:L:73:ALA:HA	1.87	0.56
1:H:83:LEU:CB	1:H:86:LEU:HD11	2.35	0.56
2:L:95:SER:O	2:L:96:ASN:CB	2.54	0.56
2:L:20:LEU:N	2:L:20:LEU:HD12	2.21	0.56
2:L:14:PRO:CG	2:L:109:LEU:O	2.54	0.56
3:P:2:PRO:C	3:P:3:TYR:HD1	2.14	0.56
1:H:32:TYR:CE2	1:H:100:ASP:HB3	2.41	0.56
1:H:194:PRO:O	1:H:198:GLU:HG2	2.06	0.56
1:H:100:ASP:OD1	1:H:106:TYR:HD1	1.88	0.55
1:H:38:LYS:HB2	1:H:48:ILE:HD11	1.89	0.55
2:L:191:HIS:HB2	2:L:194:TYR:OH	2.05	0.55
2:L:93:TRP:CD1	3:P:1:PRO:N	2.68	0.55
1:H:215:LYS:NZ	2:L:126:GLU:OE2	2.39	0.54
1:H:180:ASP:OD1	1:H:180:ASP:N	2.41	0.54
2:L:49:LEU:O	2:L:50:ILE:HD13	2.08	0.53
1:H:63:LYS:HE3	4:H:2029:HOH:O	2.07	0.53
2:L:93:TRP:HE1	3:P:2:PRO:N	2.07	0.52
3:P:2:PRO:O	3:P:3:TYR:HB3	2.09	0.52
2:L:23:ARG:HG2	2:L:72:LYS:CD	2.39	0.52
1:H:176:VAL:HG13	2:L:165:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:116:PRO:HB3	2:L:142:PHE:HB3	1.91	0.52
2:L:131:ASN:C	2:L:185:ALA:HB2	2.35	0.52
1:H:161:TRP:HE3	1:H:200:VAL:HG12	1.74	0.52
1:H:105:SER:C	1:H:106:TYR:CD1	2.89	0.51
1:H:81:MET:HE1	1:H:94:TYR:CD1	2.46	0.51
1:H:100:ASP:OD1	1:H:106:TYR:CE1	2.64	0.51
2:L:10:LEU:HD12	2:L:20:LEU:HG	1.91	0.51
2:L:93:TRP:HD1	3:P:1:PRO:H3	1.47	0.51
1:H:142:MET:HE2	1:H:189:THR:CG2	2.38	0.51
1:H:149:VAL:HG11	1:H:157:VAL:HG21	1.92	0.51
1:H:193:SER:H	1:H:194:PRO:HD2	1.74	0.51
2:L:32:SER:CB	3:P:1:PRO:HG3	2.36	0.51
2:L:151:TRP:CD1	2:L:162:MET:HG3	2.46	0.51
1:H:16:ALA:O	1:H:86:LEU:HB2	2.11	0.51
2:L:142:PHE:CE2	2:L:147:VAL:HG13	2.46	0.51
1:H:29:PHE:O	1:H:53:PRO:HG2	2.10	0.50
1:H:33:TRP:CZ2	3:P:6:TRP:HB3	2.46	0.50
2:L:51:GLY:O	2:L:55:ASN:HB2	2.11	0.50
2:L:142:PHE:CD2	2:L:147:VAL:HG13	2.47	0.50
1:H:184:LEU:CD1	1:H:185:SER:N	2.74	0.50
1:H:37:VAL:CG1	1:H:45:LEU:HD22	2.41	0.50
2:L:49:LEU:HA	2:L:60:VAL:HG21	1.94	0.50
1:H:110:TRP:HB2	2:L:46:PHE:O	2.12	0.50
1:H:152:TYR:CD2	1:H:157:VAL:CG1	2.95	0.49
1:H:178:GLN:NE2	4:H:2071:HOH:O	2.44	0.49
1:H:199:THR:HG23	1:H:200:VAL:N	2.28	0.49
1:H:177:LEU:O	2:L:163:GLU:OE2	2.31	0.49
1:H:157:VAL:HG12	1:H:206:HIS:HD2	1.74	0.49
2:L:205:VAL:HA	4:L:2066:HOH:O	2.12	0.49
1:H:30:THR:HA	1:H:53:PRO:HG2	1.95	0.48
3:P:3:TYR:CD1	3:P:3:TYR:N	2.80	0.48
2:L:123:PRO:HG2	2:L:133:ALA:HB1	1.95	0.48
2:L:158:VAL:CA	2:L:159:THR:HG22	2.39	0.48
2:L:209:LEU:C	2:L:209:LEU:HD12	2.38	0.48
1:H:152:TYR:CE2	1:H:157:VAL:CG1	2.97	0.48
2:L:170:GLN:HE21	2:L:176:MET:HB3	1.78	0.48
1:H:23:LYS:HG2	1:H:78:THR:CG2	2.44	0.48
2:L:31:THR:O	2:L:31:THR:HG23	2.13	0.48
1:H:98:ARG:O	1:H:107:PHE:O	2.32	0.48
1:H:33:TRP:CH2	3:P:6:TRP:HB3	2.49	0.47
2:L:143:TYR:CA	2:L:144:PRO:O	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:ASN:N	1:H:201:THR:O	2.47	0.47
2:L:6:GLN:HE21	2:L:101:GLY:HA3	1.79	0.47
2:L:42:PRO:HG2	4:L:2014:HOH:O	2.15	0.47
1:H:191:PRO:C	1:H:194:PRO:HD2	2.40	0.47
1:H:193:SER:N	1:H:194:PRO:CD	2.77	0.47
2:L:127:GLU:HG2	2:L:132:THR:O	2.14	0.47
3:P:2:PRO:C	3:P:3:TYR:CD1	2.92	0.47
3:P:4:PRO:HD2	3:P:6:TRP:NE1	2.30	0.47
1:H:131:LEU:HB2	1:H:146:GLY:C	2.40	0.47
1:H:194:PRO:HB2	4:H:2076:HOH:O	2.14	0.47
2:L:162:MET:HA	2:L:180:TYR:O	2.15	0.47
1:H:30:THR:HA	1:H:53:PRO:HB2	1.97	0.47
1:H:191:PRO:HG2	1:H:194:PRO:HG3	1.97	0.46
2:L:93:TRP:CZ2	2:L:96:ASN:HA	2.49	0.46
1:H:23:LYS:HG2	1:H:78:THR:HG22	1.96	0.46
2:L:209:LEU:HA	4:L:2068:HOH:O	2.15	0.46
1:H:101:TYR:N	1:H:101:TYR:CD1	2.83	0.46
2:L:95:SER:H	3:P:1:PRO:N	2.14	0.46
1:H:106:TYR:N	1:H:106:TYR:HD1	2.11	0.46
2:L:41:LYS:HB2	2:L:45:LEU:HB3	1.96	0.46
1:H:108:ASP:CG	1:H:109:TYR:H	2.23	0.46
1:H:161:TRP:HE3	1:H:200:VAL:CG1	2.28	0.46
2:L:151:TRP:HB2	2:L:158:VAL:HG12	1.97	0.46
2:L:41:LYS:HB3	2:L:42:PRO:HD2	1.96	0.46
1:H:152:TYR:CD2	1:H:157:VAL:HG11	2.51	0.45
1:H:32:TYR:HE2	1:H:100:ASP:HB3	1.82	0.45
2:L:207:LYS:HD3	2:L:207:LYS:HA	1.76	0.45
2:L:6:GLN:NE2	2:L:90:CYS:N	2.64	0.45
1:H:2:VAL:HB	1:H:109:TYR:CE2	2.52	0.44
3:P:3:TYR:HD1	3:P:3:TYR:N	2.15	0.44
2:L:83:ASP:O	2:L:87:TYR:OH	2.29	0.44
1:H:15:GLY:N	1:H:86:LEU:O	2.39	0.44
2:L:69:ILE:HG12	2:L:74:ALA:HB3	1.99	0.44
2:L:24:SER:HB3	2:L:29:VAL:HG22	2.00	0.44
1:H:209:SER:O	1:H:210:SER:C	2.61	0.43
2:L:143:TYR:CD1	2:L:144:PRO:HA	2.53	0.43
2:L:137:CYS:O	2:L:178:SER:HA	2.18	0.43
2:L:210:SER:N	4:L:2068:HOH:O	2.51	0.43
1:H:4:LEU:HA	1:H:23:LYS:O	2.18	0.43
1:H:58:THR:HG1	1:H:60:TYR:HE2	1.63	0.43
3:P:3:TYR:CG	3:P:4:PRO:HD3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:TRP:HA	1:H:95:TYR:O	2.19	0.42
1:H:170:VAL:HA	1:H:187:SER:O	2.20	0.42
1:H:29:PHE:CD2	1:H:77:SER:HA	2.55	0.42
1:H:108:ASP:OD2	1:H:109:TYR:HD1	2.03	0.42
1:H:178:GLN:OE1	2:L:163:GLU:CG	2.67	0.42
2:L:63:ARG:HB2	2:L:77:THR:O	2.20	0.42
1:H:5:GLN:HG2	1:H:23:LYS:CB	2.49	0.42
1:H:199:THR:HG23	1:H:200:VAL:H	1.83	0.42
2:L:6:GLN:HE22	2:L:90:CYS:N	2.16	0.42
2:L:135:LEU:HB2	2:L:181:LEU:HB3	2.01	0.42
2:L:4:VAL:CG1	2:L:22:CYS:SG	3.08	0.41
1:H:199:THR:HG21	1:H:216:ALA:HB1	2.01	0.41
2:L:14:PRO:HD3	2:L:109:LEU:O	2.19	0.41
1:H:47:TRP:O	1:H:61:ASN:ND2	2.53	0.41
1:H:60:TYR:CE1	1:H:70:LEU:HG	2.55	0.41
1:H:50:ARG:NH1	3:P:3:TYR:CE2	2.87	0.41
1:H:5:GLN:HG2	1:H:23:LYS:HB3	2.02	0.41
1:H:188:VAL:O	1:H:188:VAL:HG13	2.20	0.41
1:H:101:TYR:HB2	3:P:6:TRP:HB2	2.02	0.41
1:H:30:THR:HA	1:H:53:PRO:CB	2.51	0.41
1:H:168:SER:C	1:H:170:VAL:N	2.76	0.41
2:L:39:GLN:CD	2:L:41:LYS:HZ3	2.29	0.41
2:L:60:VAL:HG12	2:L:61:PRO:O	2.20	0.41
1:H:36:TRP:NE1	4:H:2021:HOH:O	2.40	0.41
1:H:160:THR:OG1	1:H:203:ASN:HB2	2.20	0.41
1:H:161:TRP:HB2	1:H:166:LEU:HB2	2.03	0.41
2:L:154:ASP:OD2	2:L:191:HIS:HD2	2.04	0.41
3:P:2:PRO:HA	3:P:6:TRP:HZ2	1.86	0.41
1:H:194:PRO:O	1:H:198:GLU:O	2.39	0.40
2:L:93:TRP:HB2	2:L:98:TRP:CZ3	2.56	0.40
1:H:191:PRO:HG2	1:H:194:PRO:CD	2.51	0.40
1:H:161:TRP:CE3	1:H:200:VAL:CG1	3.05	0.40
2:L:32:SER:HA	2:L:34:TYR:CE1	2.57	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	H	211/220 (96%)	193 (92%)	13 (6%)	5 (2%)	4	5
2	L	209/211 (99%)	195 (93%)	13 (6%)	1 (0%)	24	37
3	P	4/12 (33%)	1 (25%)	0	3 (75%)	0	0
All	All	424/443 (96%)	389 (92%)	26 (6%)	9 (2%)	5	7

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	108	ASP
1	H	156	PRO
1	H	197	SER
2	L	96	ASN
3	P	2	PRO
3	P	3	TYR
3	P	4	PRO
1	H	105	SER
1	H	104	GLY

5.3.2 Protein sidechains [i](#)

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	H	180/183 (98%)	157 (87%)	23 (13%)	4	6
2	L	177/177 (100%)	164 (93%)	13 (7%)	13	22
3	P	5/9 (56%)	3 (60%)	2 (40%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	362/369 (98%)	324 (90%)	38 (10%)	6 10

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLN
1	H	3	GLN
1	H	13	LYS
1	H	23	LYS
1	H	50	ARG
1	H	52	ASP
1	H	71	THR
1	H	78	THR
1	H	86	LEU
1	H	98	ARG
1	H	102	TYR
1	H	105	SER
1	H	106	TYR
1	H	142	MET
1	H	155	GLU
1	H	163	SER
1	H	166	LEU
1	H	167	SER
1	H	180	ASP
1	H	198	GLU
1	H	199	THR
1	H	210	SER
1	H	215	LYS
2	L	1	GLN
2	L	5	THR
2	L	31	THR
2	L	36	ASN
2	L	45	LEU
2	L	77	THR
2	L	81	THR
2	L	126	GLU
2	L	169	LYS
2	L	188	TRP
2	L	192	SER
2	L	197	GLN
2	L	204	THR
3	P	2	PRO

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Mol	Chain	Res	Type
3	P	3	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	1	GLN
1	H	5	GLN
1	H	6	GLN
1	H	203	ASN
2	L	6	GLN
2	L	36	ASN
2	L	160	GLN
2	L	170	GLN
2	L	173	ASN
2	L	200	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	215/220 (97%)	0.33	9 (4%) 40 36	26, 37, 54, 59	0
2	L	211/211 (100%)	0.16	2 (0%) 81 78	24, 34, 44, 51	0
3	P	6/12 (50%)	1.39	1 (16%) 4 3	36, 38, 38, 39	0
All	All	432/443 (97%)	0.26	12 (2%) 55 51	24, 36, 51, 59	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	15	GLY	2.8
1	H	104	GLY	2.7
1	H	102	TYR	2.7
1	H	103	GLY	2.6
1	H	53	PRO	2.5
1	H	156	PRO	2.3
1	H	134	GLY	2.3
1	H	101	TYR	2.3
2	L	76	ILE	2.2
1	H	105	SER	2.2
3	P	6	TRP	2.1
1	H	195	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.