



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:18 PM UTC

PDB ID : 9HK1 / pdb_00009hk1
Title : PD1 signaling receptor bound to FAB Complex
Authors : Bjorkelid, C.; Paluch, C.; Robertson, N.J.
Deposited on : 2024-12-02
Resolution : 2.03 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	:	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

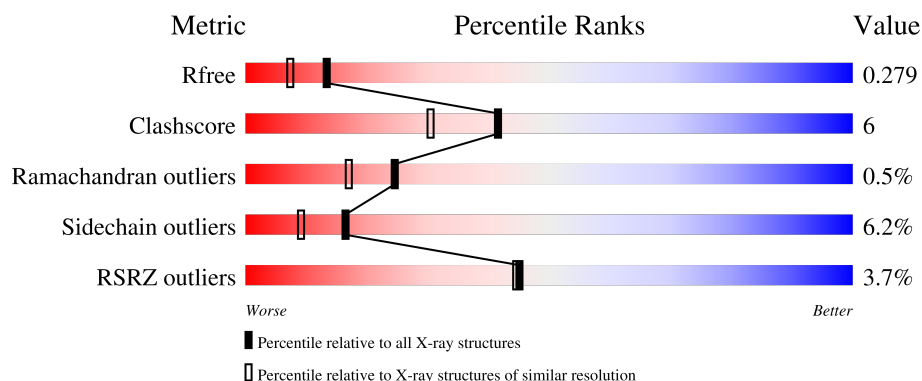
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	A	129	<div> <div>9%</div> <div>60%</div> <div>15%</div> <div>5%</div> <div>20%</div> </div>
1	B	129	<div> <div>8%</div> <div>60%</div> <div>17%</div> <div>..</div> <div>19%</div> </div>
2	L	215	<div> <div>84%</div> <div>13%</div> <div>..</div> </div>
2	M	215	<div> <div>82%</div> <div>15%</div> <div>..</div> </div>
3	H	227	<div> <div>4%</div> <div>78%</div> <div>15%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	227	<div><div></div><div>3%</div><div>78%</div><div>14%</div><div>• 6%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8487 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 Programmed cell death protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			821	513	151	153	4			
1	B	104	Total	C	N	O	S	0	0	0
			830	518	150	158	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q15116
A	2	PRO	-	expression tag	UNP Q15116
A	3	SER	-	expression tag	UNP Q15116
A	4	GLY	-	expression tag	UNP Q15116
A	5	ALA	-	expression tag	UNP Q15116
A	74	SER	CYS	conflict	UNP Q15116
B	1	GLY	-	expression tag	UNP Q15116
B	2	PRO	-	expression tag	UNP Q15116
B	3	SER	-	expression tag	UNP Q15116
B	4	GLY	-	expression tag	UNP Q15116
B	5	ALA	-	expression tag	UNP Q15116
B	74	SER	CYS	conflict	UNP Q15116

- Molecule 2 is a protein called Antibody FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1629	1020	272	333	4			
2	M	212	Total	C	N	O	S	0	1	0
			1632	1022	272	334	4			

- Molecule 3 is a protein called Antibody FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	214	Total	C	N	O	S	0	0	0
			1630	1038	268	318	6			
3	I	213	Total	C	N	O	S	0	0	0
			1624	1035	267	316	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total	O	0	0
			15	15		
5	B	13	Total	O	0	0
			13	13		
5	L	72	Total	O	0	0
			72	72		
5	H	67	Total	O	0	0
			67	67		
5	M	70	Total	O	0	0
			70	70		

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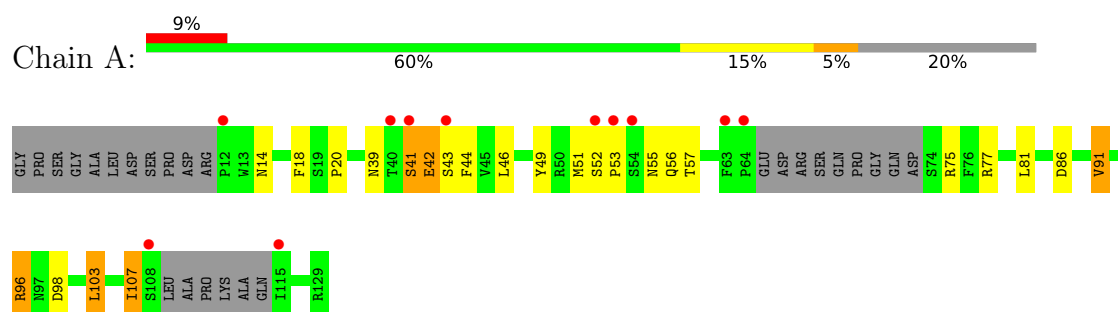
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	56	Total	O	0	0
			56	56		

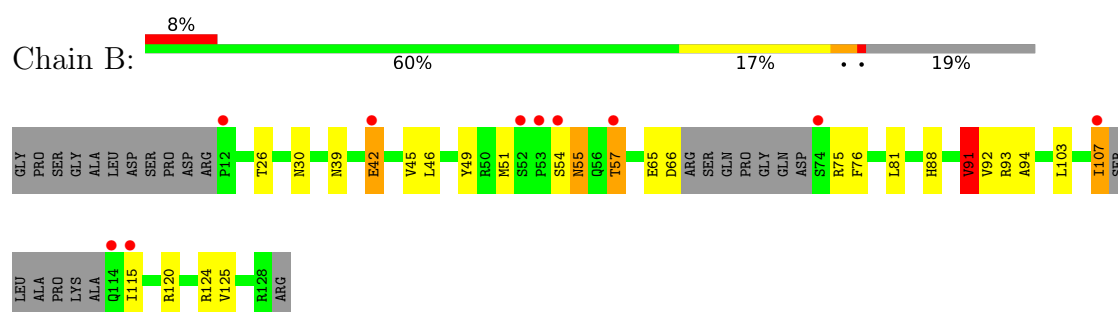
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

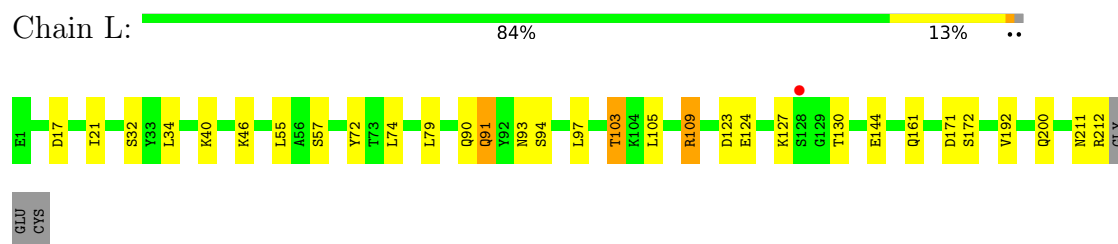
- Molecule 1: Programmed cell death protein 1



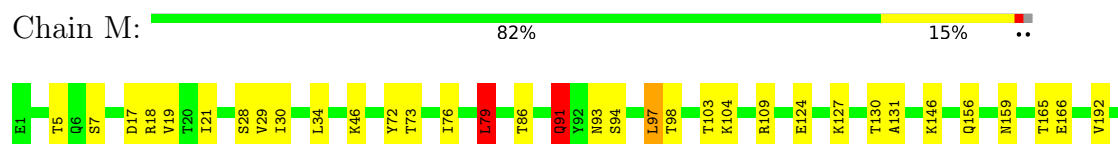
- Molecule 1: Programmed cell death protein 1

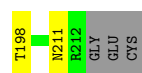


- Molecule 2: Antibody FAB light chain

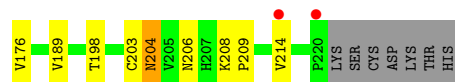
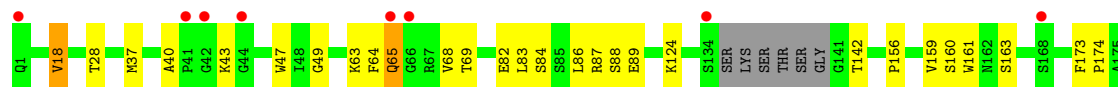
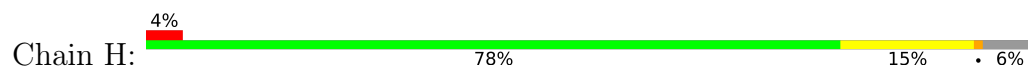


- Molecule 2: Antibody FAB light chain

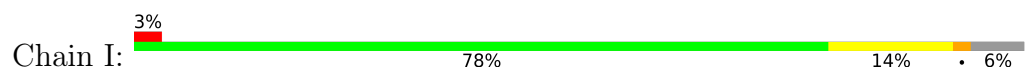




• Molecule 3: Antibody FAB heavy chain



• Molecule 3: Antibody FAB heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.16Å 53.79Å 103.00Å 104.80° 101.83° 92.57°	Depositor
Resolution (Å)	51.85 – 2.03 51.85 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.0 (51.85-2.03) 98.1 (51.85-2.03)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.210 , 0.276 0.214 , 0.279	Depositor DCC
R_{free} test set	3095 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-h-k-l 0.036 for -k,-h,-l 0.007 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8487	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.61	0/839	1.21	6/1135 (0.5%)
1	B	0.59	0/848	1.22	3/1148 (0.3%)
2	L	0.67	0/1665	1.24	9/2263 (0.4%)
2	M	0.66	0/1671	1.17	9/2272 (0.4%)
3	H	0.60	0/1673	1.14	4/2280 (0.2%)
3	I	0.62	0/1667	1.17	5/2272 (0.2%)
All	All	0.63	0/8363	1.19	36/11370 (0.3%)

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	B	0	1
3	H	0	1
3	I	0	2
All	All	0	4

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	91	GLN	N-CA-CB	-8.43	96.16	110.83
2	L	109	ARG	N-CA-CB	-7.55	99.83	111.46
2	M	109	ARG	N-CA-CB	-7.50	99.92	111.46
2	M	127	LYS	CB-CA-C	-7.44	98.44	110.79
1	B	42	GLU	CB-CG-CD	7.28	124.97	112.60
2	L	17	ASP	CA-CB-CG	7.18	119.78	112.60
3	I	64	PHE	CA-CB-CG	7.18	120.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	VAL	N-CA-CB	6.30	119.82	111.25
1	A	96	ARG	CB-CA-C	-6.28	101.02	110.88
1	B	26	THR	CA-CB-OG1	-6.22	100.27	109.60
1	A	96	ARG	N-CA-CB	6.19	118.98	110.01
2	M	46	LYS	CB-CA-C	6.16	120.85	109.70
1	A	18	PHE	CA-CB-CG	6.08	119.88	113.80
3	I	18	VAL	N-CA-CB	5.97	121.23	111.44
2	M	79	LEU	N-CA-CB	-5.95	100.58	109.69
2	L	40	LYS	CB-CA-C	5.92	118.79	109.37
2	L	130	THR	CA-CB-OG1	-5.92	100.72	109.60
2	M	86	THR	CA-CB-OG1	-5.86	100.82	109.60
2	M	91	GLN	CB-CA-C	5.85	120.54	109.37
2	L	127	LYS	CB-CA-C	-5.77	100.87	110.68
1	B	91	VAL	N-CA-CB	5.70	117.83	110.99
3	H	142	THR	CA-CB-OG1	-5.69	101.07	109.60
2	L	103	THR	CA-CB-OG1	-5.57	101.24	109.60
2	L	46	LYS	CB-CA-C	5.50	119.65	109.70
2	M	165	THR	CA-CB-OG1	-5.48	101.38	109.60
1	A	42	GLU	N-CA-CB	5.40	119.61	110.49
3	I	158	THR	CA-CB-OG1	-5.31	101.64	109.60
2	M	124	GLU	CB-CG-CD	5.30	121.61	112.60
1	A	14	ASN	O-C-N	-5.29	119.10	121.53
3	H	69	THR	CA-CB-OG1	-5.27	101.69	109.60
2	L	109	ARG	CG-CD-NE	-5.25	100.44	112.00
2	M	109	ARG	CG-CD-NE	-5.20	100.55	112.00
3	H	206	ASN	CB-CA-C	-5.18	100.23	109.71
3	H	28	THR	CA-CB-OG1	-5.14	101.89	109.60
3	I	18	VAL	CB-CA-C	-5.11	102.63	110.50
3	I	69	THR	CA-CB-OG1	-5.06	102.02	109.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	124	ARG	Sidechain
3	H	87	ARG	Sidechain
3	I	66	GLY	Peptide
3	I	98	ARG	Sidechain

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	A	821	0	797	24	0
1	B	830	0	797	16	0
2	L	1629	0	1584	17	0
2	M	1632	0	1589	20	0
3	H	1630	0	1588	13	0
3	I	1624	0	1583	16	0
4	A	14	0	13	5	0
4	B	14	0	13	4	0
5	A	15	0	0	0	0
5	B	13	0	0	1	0
5	H	67	0	0	1	0
5	I	56	0	0	1	0
5	L	72	0	0	0	0
5	M	70	0	0	0	0
All	All	8487	0	7964	104	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 6.

All (104) 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:30:ASN:HD21	4:B:201:NAG:C1	1.78	0.96
2:M:34:LEU:HD22	2:M:72:TYR:CG	2.09	0.87
2:L:91:GLN:HE22	2:L:94:SER:H	1.14	0.87
2:L:91:GLN:NE2	2:L:94:SER:H	1.81	0.79
2:M:21:ILE:HD12	2:M:103:THR:HG21	1.64	0.79
2:L:21:ILE:HD12	2:L:103:THR:HG21	1.66	0.78
1:A:51:MET:HE1	1:A:57:THR:HG22	1.67	0.76
1:A:39:ASN:HD21	4:A:201:NAG:C1	1.99	0.76
3:I:210:SER:OG	3:I:212:THR:OG1	2.07	0.73
2:L:34:LEU:HD22	2:L:72:TYR:CG	2.23	0.72
1:B:39:ASN:ND2	5:B:301:HOH:O	2.22	0.72
3:H:40:ALA:HB3	3:H:43:LYS:HG3	1.74	0.69
1:A:51:MET:HE3	1:A:103:LEU:HD22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:34:LEU:CD2	2:M:72:TYR:CG	2.76	0.68
3:I:18:VAL:HG22	3:I:86:LEU:HD11	1.76	0.67
2:M:156:GLN:HE21	2:M:159:ASN:HD21	1.43	0.67
1:A:96:ARG:HH12	2:L:93:ASN:ND2	1.95	0.65
1:A:51:MET:HE3	1:A:103:LEU:CD2	2.27	0.64
2:M:34:LEU:HD22	2:M:72:TYR:CD2	2.33	0.63
1:A:42:GLU:HB3	4:A:201:NAG:H82	1.80	0.62
1:A:51:MET:HE1	1:A:57:THR:CG2	2.30	0.62
1:B:30:ASN:ND2	4:B:201:NAG:C1	2.59	0.62
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.35	0.61
1:A:77:ARG:HH11	1:A:77:ARG:HG3	1.66	0.60
1:A:81:LEU:HD12	1:A:86:ASP:HB3	1.85	0.59
2:M:19:VAL:HG22	2:M:76:ILE:HB	1.85	0.58
3:H:160:SER:OG	3:H:204:ASN:ND2	2.21	0.58
2:M:91:GLN:NE2	2:M:94:SER:H	2.01	0.57
3:H:163:SER:H	3:H:204:ASN:HD21	1.51	0.57
3:H:89:GLU:HG3	5:H:327:HOH:O	2.04	0.56
1:B:54:SER:O	1:B:55:ASN:HB2	2.06	0.56
1:B:30:ASN:HD21	4:B:201:NAG:C2	2.18	0.55
3:H:18:VAL:HG22	3:H:86:LEU:HD11	1.89	0.55
3:I:154:PRO:O	3:I:207:HIS:HE1	1.89	0.54
1:A:49:TYR:HB2	1:A:103:LEU:CD2	2.38	0.54
2:M:104:LYS:NZ	2:M:166:GLU:OE1	2.37	0.53
2:L:91:GLN:HE21	2:L:93:ASN:H	1.57	0.53
3:H:64:PHE:O	3:H:65:GLN:C	2.52	0.53
1:A:44:PHE:HA	1:A:107:ILE:O	2.09	0.52
1:A:49:TYR:HB2	1:A:103:LEU:HD23	1.92	0.52
1:B:76:PHE:CE2	1:B:91:VAL:HG13	2.45	0.51
2:M:192:VAL:HG22	2:M:211:ASN:HD22	1.76	0.51
1:A:41:SER:O	1:A:42:GLU:HG2	2.10	0.51
2:M:34:LEU:HD22	2:M:72:TYR:CD1	2.45	0.51
3:I:191:VAL:HG11	3:I:201:TYR:CE1	2.46	0.51
3:I:9:ALA:HB2	5:I:328:HOH:O	2.11	0.50
1:A:51:MET:CE	1:A:57:THR:HG22	2.40	0.50
2:L:192:VAL:HG22	2:L:211:ASN:OD1	2.11	0.49
2:M:156:GLN:NE2	2:M:159:ASN:HD21	2.08	0.49
1:A:42:GLU:N	4:A:201:NAG:H83	2.28	0.49
1:B:51:MET:HE2	1:B:120:ARG:HH22	1.78	0.49
1:B:65:GLU:O	1:B:66:ASP:HB2	2.12	0.49
3:H:68:VAL:HG22	3:H:83:LEU:HD13	1.96	0.48
1:A:52:SER:HB2	1:A:53:PRO:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:SER:CB	1:A:53:PRO:CD	2.92	0.47
2:M:30:ILE:H	2:M:93:ASN:ND2	2.13	0.47
2:L:90:GLN:HG2	2:L:91:GLN:N	2.30	0.46
1:A:42:GLU:HB3	4:A:201:NAG:C8	2.45	0.46
1:A:52:SER:CB	1:A:53:PRO:HD2	2.45	0.46
3:I:37:MET:HE3	3:I:110:TRP:CZ3	2.51	0.46
2:L:144:GLU:CD	2:L:144:GLU:H	2.24	0.45
2:L:171:ASP:O	2:L:172:SER:HB2	2.16	0.45
3:H:208:LYS:N	3:H:209:PRO:CD	2.79	0.45
2:M:146:LYS:HB3	2:M:198:THR:HB	1.99	0.44
1:B:75:ARG:HD2	1:B:92:VAL:O	2.17	0.44
1:B:30:ASN:HD21	4:B:201:NAG:H2	1.82	0.44
3:H:68:VAL:HA	3:H:82:GLU:O	2.18	0.44
3:H:159:VAL:HA	3:H:204:ASN:O	2.17	0.43
3:I:208:LYS:N	3:I:209:PRO:CD	2.81	0.43
2:L:34:LEU:HD22	2:L:72:TYR:CD2	2.54	0.43
2:L:91:GLN:HE21	2:L:93:ASN:N	2.16	0.43
3:I:191:VAL:HG11	3:I:201:TYR:CZ	2.53	0.43
1:B:49:TYR:CD2	1:B:57:THR:HG23	2.53	0.43
1:B:94:ALA:HB1	1:B:125:VAL:HG21	2.00	0.43
3:I:12:LYS:HE3	3:I:18:VAL:HG13	1.99	0.43
2:M:97:LEU:HD22	3:I:47:TRP:NE1	2.34	0.43
1:A:77:ARG:HG3	1:A:77:ARG:NH1	2.33	0.43
3:H:161:TRP:CH2	3:H:203:CYS:HB3	2.54	0.43
1:A:39:ASN:ND2	4:A:201:NAG:C1	2.74	0.42
1:B:45:VAL:O	1:B:107:ILE:HD12	2.20	0.42
3:I:207:HIS:HD2	3:I:210:SER:OG	2.02	0.42
1:A:81:LEU:HD12	1:A:86:ASP:CB	2.50	0.42
3:I:185:LEU:C	3:I:185:LEU:HD12	2.44	0.42
1:A:75:ARG:HH12	1:A:98:ASP:CG	2.27	0.42
1:B:81:LEU:HD21	1:B:88:HIS:CD2	2.55	0.42
1:B:103:LEU:HD23	1:B:103:LEU:N	2.35	0.41
2:L:123:ASP:O	2:L:124:GLU:C	2.63	0.41
2:L:91:GLN:NE2	2:L:93:ASN:H	2.17	0.41
1:A:52:SER:HB2	1:A:53:PRO:HD2	2.02	0.41
3:H:173:PHE:O	3:H:174:PRO:C	2.62	0.41
2:M:18:ARG:HA	2:M:76:ILE:O	2.20	0.41
3:I:18:VAL:O	3:I:82:GLU:HA	2.20	0.41
2:M:19:VAL:HG21	2:M:76:ILE:HD12	2.02	0.41
2:M:91:GLN:OE1	2:M:98:THR:OG1	2.33	0.41
3:I:175:ALA:HA	3:I:185:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:79:LEU:HD21	2:L:105:LEU:HD21	2.01	0.41
2:L:91:GLN:NE2	2:L:93:ASN:N	2.69	0.41
2:M:17:ASP:O	2:M:79:LEU:HB2	2.21	0.41
2:M:130:THR:HG22	2:M:131:ALA:N	2.36	0.41
2:M:192:VAL:HG22	2:M:211:ASN:ND2	2.36	0.41
3:I:128:VAL:O	3:I:216:LYS:HD2	2.21	0.41
3:I:24:ALA:HB1	3:I:27:TYR:CE1	2.56	0.40
1:B:51:MET:HE2	1:B:120:ARG:NH2	2.37	0.40
2:L:212:ARG:HG2	2:L:212:ARG:HH11	1.86	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	97/129 (75%)	90 (93%)	6 (6%)	1 (1%)	12	5
1	B	98/129 (76%)	95 (97%)	2 (2%)	1 (1%)	12	5
2	L	210/215 (98%)	205 (98%)	5 (2%)	0	100	100
2	M	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
3	H	210/227 (92%)	203 (97%)	6 (3%)	1 (0%)	24	17
3	I	209/227 (92%)	198 (95%)	9 (4%)	2 (1%)	12	5
All	All	1035/1142 (91%)	996 (96%)	34 (3%)	5 (0%)	24	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	B	55	ASN
3	H	65	GLN

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Mol	Chain	Res	Type
3	I	151	ASP
3	I	198	THR

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	92/112 (82%)	84 (91%)	8 (9%)	9	4
1	B	93/112 (83%)	86 (92%)	7 (8%)	12	7
2	L	188/190 (99%)	180 (96%)	8 (4%)	26	19
2	M	189/190 (100%)	181 (96%)	8 (4%)	26	20
3	H	183/195 (94%)	171 (93%)	12 (7%)	15	8
3	I	182/195 (93%)	168 (92%)	14 (8%)	12	6
All	All	927/994 (93%)	870 (94%)	57 (6%)	16	10

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PRO
1	A	41	SER
1	A	46	LEU
1	A	55	ASN
1	A	56	GLN
1	A	91	VAL
1	A	103	LEU
1	A	107	ILE
1	B	42	GLU
1	B	46	LEU
1	B	57	THR
1	B	91	VAL
1	B	93	ARG
1	B	107	ILE
1	B	115	ILE
2	L	32	SER

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Mol	Chain	Res	Type
2	L	55	LEU
2	L	57	SER
2	L	74	LEU
2	L	97	LEU
2	L	109	ARG
2	L	161	GLN
2	L	200	GLN
3	H	18	VAL
3	H	37	MET
3	H	63	LYS
3	H	84	SER
3	H	88	SER
3	H	124	LYS
3	H	156	PRO
3	H	176	VAL
3	H	189	VAL
3	H	198	THR
3	H	204	ASN
3	H	214	VAL
2	M	5	THR
2	M	7	SER
2	M	28	SER
2	M	29	VAL
2	M	73	THR
2	M	79	LEU
2	M	91	GLN
2	M	97	LEU
3	I	18	VAL
3	I	37	MET
3	I	62	GLU
3	I	63	LYS
3	I	64	PHE
3	I	85	SER
3	I	88	SER
3	I	156	PRO
3	I	179	SER
3	I	204	ASN
3	I	206	ASN
3	I	208	LYS
3	I	212	THR
3	I	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	88	HIS
1	B	30	ASN
1	B	47	ASN
1	B	55	ASN
1	B	88	HIS
2	L	38	GLN
2	L	91	GLN
2	L	93	ASN
3	H	65	GLN
3	H	178	GLN
3	H	204	ASN
3	H	206	ASN
2	M	3	GLN
2	M	39	GLN
2	M	54	ASN
2	M	91	GLN
2	M	156	GLN
2	M	211	ASN
3	I	39	GLN
3	I	65	GLN
3	I	199	GLN
3	I	207	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](#)

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	$\# Z > 2$
4	NAG	B	201	-	14,14,15	0.50	0	17,19,21	1.46	2 (11%)
4	NAG	A	201	-	14,14,15	0.37	0	17,19,21	1.69	4 (23%)

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
4	NAG	B	201	-	-	4/6/23/26	0/1/1/1
4	NAG	A	201	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	201	NAG	C1-C2-N2	4.61	117.70	110.43
4	A	201	NAG	O5-C1-C2	-4.07	104.99	111.29
4	A	201	NAG	C1-C2-N2	3.36	115.73	110.43
4	B	201	NAG	O5-C1-C2	-3.23	106.29	111.29
4	A	201	NAG	C2-N2-C7	3.01	126.94	122.90
4	A	201	NAG	C4-C3-C2	-2.34	107.59	111.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	201	NAG	C8-C7-N2-C2
4	B	201	NAG	O7-C7-N2-C2
4	B	201	NAG	O5-C5-C6-O6
4	B	201	NAG	C4-C5-C6-O6
4	A	201	NAG	C8-C7-N2-C2
4	A	201	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	201	NAG	4	0
4	A	201	NAG	5	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 ⓘ

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	A	103/129 (79%)	0.79	11 (10%) 11 10	26, 42, 76, 109	0
1	B	104/129 (80%)	0.64	10 (9%) 13 12	21, 39, 71, 89	0
2	L	212/215 (98%)	0.03	1 (0%) 87 87	21, 31, 44, 59	0
2	M	212/215 (98%)	0.03	0 100 100	19, 30, 44, 56	1 (0%)
3	H	214/227 (94%)	0.32	10 (4%) 36 35	21, 33, 55, 74	0
3	I	213/227 (93%)	0.25	7 (3%) 49 48	21, 32, 53, 77	0
All	All	1058/1142 (92%)	0.27	39 (3%) 45 44	19, 33, 55, 109	1 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	PRO	3.7
3	H	65	GLN	3.7
1	B	107	ILE	3.5
3	I	198	THR	3.2
1	B	12	PRO	3.2
1	A	53	PRO	3.0
3	H	220	PRO	3.0
3	I	121	ALA	2.9
1	A	12	PRO	2.9
3	I	41	PRO	2.9
1	A	41	SER	2.9
3	H	1	GLN	2.7
3	H	41	PRO	2.7
3	I	1	GLN	2.6
1	A	40	THR	2.6
1	B	57	THR	2.5
1	A	43	SER	2.5
1	B	115	ILE	2.5
1	A	115	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	54	SER	2.5
1	B	74	SER	2.4
3	H	134	SER	2.4
1	B	114	GLN	2.4
3	H	66	GLY	2.4
3	H	44	GLY	2.3
1	A	108	SER	2.3
1	A	52	SER	2.3
3	I	65	GLN	2.2
1	A	64	PRO	2.2
3	H	214	VAL	2.2
3	H	168	SER	2.2
1	A	54	SER	2.2
2	L	128	SER	2.2
1	B	42	GLU	2.1
3	H	42	GLY	2.1
3	I	141	GLY	2.1
1	A	63	PHE	2.1
3	I	64	PHE	2.1
1	B	52	SER	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	201	14/15	0.70	0.16	55,64,76,90	0
4	NAG	B	201	14/15	0.79	0.15	48,60,70,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.