



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:28 AM GMT

PDB ID : 2H9G
Title : Crystal structure of phage derived Fab BdF1 with human Death Receptor 5 (DR5)
Authors : Hymowitz, S.G.; Compaaan, D.M.
Deposited on : 2006-06-09
Resolution : 2.32 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

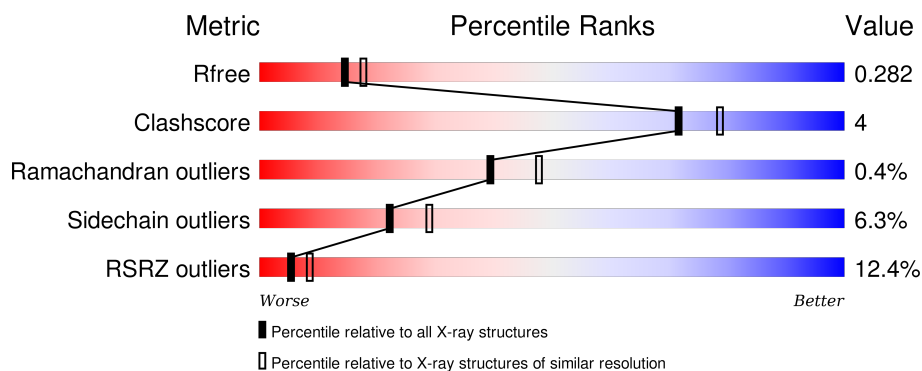
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	214	<div> <div>3%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	L	214	<div> <div>10%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
2	B	228	<div> <div>3%</div> <div>83%</div> <div>9%</div> <div>6%</div> </div>
2	H	228	<div> <div>5%</div> <div>82%</div> <div>9%</div> <div>6%</div> </div>
3	R	130	<div> <div>35%</div> <div>72%</div> <div>7%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
3	S	130	<p>26% 42% 5% 51%</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7899 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 Fab BdF1, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	L	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			

- Molecule 2 is a protein called Fab BdF1, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1600	1012	273	308	7			
2	H	215	Total	C	N	O	S	0	0	0
			1600	1012	273	308	7			

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 10B precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	108	Total	C	N	O	S	35	0	0
			833	498	150	169	16			
3	S	64	Total	C	N	O	S	69	0	0
			489	293	87	101	8			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	49	Total	O	0	0
			49	49		
4	H	31	Total	O	0	0
			31	31		
4	L	27	Total	O	0	0
			27	27		

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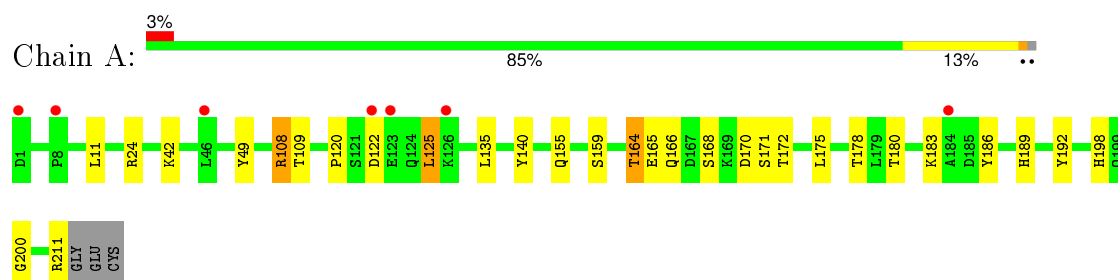
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	4	Total	O	0	0
			4	4		

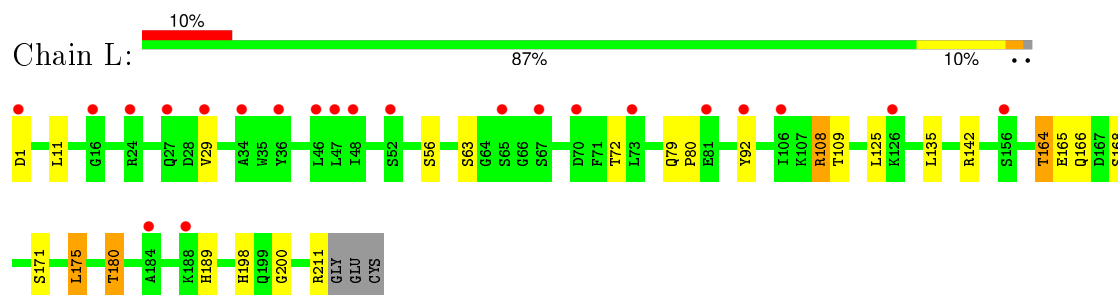
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

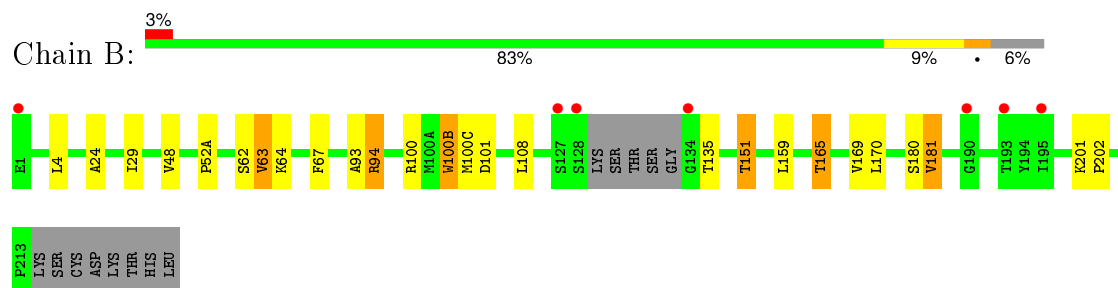
- Molecule 1: Fab Bdf1, light chain



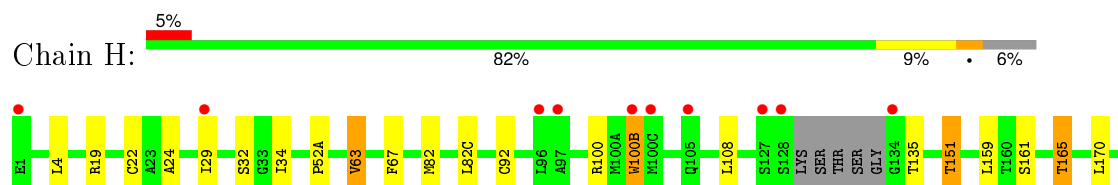
- Molecule 1: Fab Bdf1, light chain



- Molecule 2: Fab Bdf1, heavy chain

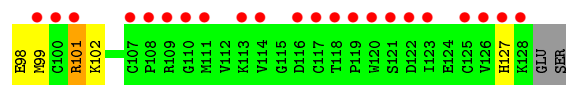
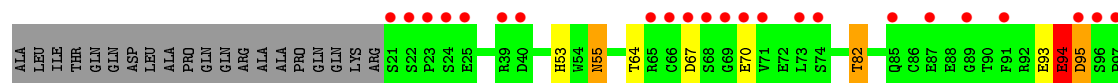


- Molecule 2: Fab Bdf1, heavy chain

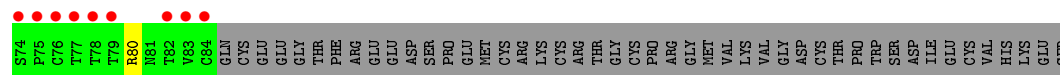
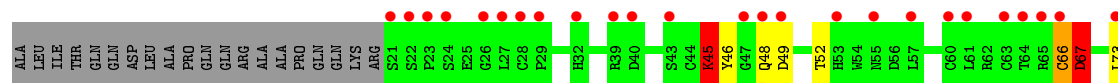
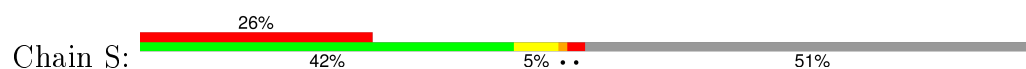




- Molecule 3: Tumor necrosis factor receptor superfamily member 10B precursor



- Molecule 3: Tumor necrosis factor receptor superfamily member 10B precursor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.81Å 61.39Å 108.27Å 90.00° 101.17° 90.00°	Depositor
Resolution (Å)	30.00 – 2.32 29.63 – 2.32	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.00-2.32) 97.0 (29.63-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.228 , 0.282 0.232 , 0.282	Depositor DCC
R_{free} test set	5485 reflections (11.21%)	DCC
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 54443 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7899	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	A	0.50	0/1653	0.65	0/2248
1	L	0.46	0/1653	0.61	1/2248 (0.0%)
2	B	0.63	1/1638 (0.1%)	0.67	0/2233
2	H	0.58	1/1638 (0.1%)	0.65	0/2233
3	R	1.39	5/851 (0.6%)	0.98	8/1150 (0.7%)
3	S	0.89	3/500 (0.6%)	1.74	7/679 (1.0%)
All	All	0.71	10/7933 (0.1%)	0.80	16/10791 (0.1%)

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
3	R	0	1
3	S	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	94	GLU	CB-CG	-21.24	1.11	1.52
3	R	95	ASP	CB-CG	19.95	1.93	1.51
3	R	93	GLU	CB-CG	16.66	1.83	1.52
3	S	66	CYS	C-N	-16.31	0.96	1.34
2	B	100(B)	TRP	C-N	14.57	1.67	1.34
3	R	101	ARG	CB-CG	-14.12	1.14	1.52
2	H	100(B)	TRP	C-N	13.94	1.66	1.34
3	R	99	MET	CB-CG	10.91	1.86	1.51
3	S	80	ARG	CB-CG	-5.72	1.37	1.52
3	S	45	LYS	CB-CG	5.20	1.66	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	66	CYS	O-C-N	-36.03	65.05	122.70
3	R	94	GLU	CB-CG-CD	-12.66	80.02	114.20
3	R	98	GLU	CA-CB-CG	12.51	140.91	113.40
3	S	66	CYS	CA-C-N	12.48	144.67	117.20
3	S	46	TYR	CB-CG-CD1	-10.13	114.92	121.00
3	S	66	CYS	C-N-CA	9.74	146.05	121.70
3	S	46	TYR	CB-CG-CD2	9.38	126.63	121.00
3	R	95	ASP	CB-CG-OD2	8.97	126.38	118.30
3	R	95	ASP	CB-CG-OD1	-8.79	110.39	118.30
3	R	102	LYS	CA-CB-CG	7.43	129.76	113.40
3	R	101	ARG	CA-CB-CG	7.43	129.75	113.40
3	S	80	ARG	CA-CB-CG	7.12	129.06	113.40
3	R	95	ASP	CA-CB-CG	-6.54	99.02	113.40
3	R	101	ARG	CB-CG-CD	5.54	126.02	111.60
3	S	67	ASP	CB-CG-OD1	5.35	123.11	118.30
1	L	175	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	R	95	ASP	Sidechain
3	S	66	CYS	Mainchain

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	1617	0	1573	16	0
1	L	1617	0	1573	12	0
2	B	1600	0	1582	18	0
2	H	1600	0	1582	15	0
3	R	833	0	755	4	0
3	S	489	0	437	1	0
4	A	32	0	0	2	0
4	B	49	0	0	4	0
4	H	31	0	0	2	0
4	L	27	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	4	0	0	0	0
All	All	7899	0	7502	63	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 4.

All (63) 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:B:100(B):TRP:C	2:B:100(C):MET:N	1.67	1.43
2:H:22:CYS:HG	2:H:92:CYS:HG	0.97	0.78
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.76	0.68
2:B:100(B):TRP:C	2:B:100(C):MET:CA	2.62	0.67
2:H:151:THR:HG22	4:H:237:HOH:O	2.00	0.62
2:H:165:THR:HG22	2:H:180:SER:OG	2.00	0.61
1:L:198:HIS:CD2	1:L:200:GLY:H	2.18	0.61
1:A:198:HIS:CD2	1:A:200:GLY:H	2.19	0.61
2:B:29:ILE:HG22	2:B:52(A):PRO:HG2	1.84	0.59
1:A:135:LEU:HD22	2:B:181:VAL:HG21	1.86	0.57
1:A:108:ARG:HD3	1:A:109:THR:O	2.05	0.57
1:A:164:THR:CG2	4:A:215:HOH:O	2.52	0.57
1:L:189:HIS:O	1:L:211:ARG:NH1	2.39	0.56
1:L:29:VAL:HG13	1:L:92:TYR:HB2	1.87	0.56
2:B:63:VAL:HG13	2:B:67:PHE:HB2	1.89	0.55
2:B:165:THR:HG22	2:B:180:SER:OG	2.07	0.55
2:B:29:ILE:CG2	2:B:52(A):PRO:HG2	2.37	0.54
1:L:164:THR:CG2	4:L:215:HOH:O	2.55	0.54
1:L:164:THR:HG21	4:L:215:HOH:O	2.07	0.54
1:L:164:THR:HG23	1:L:165:GLU:O	2.08	0.53
2:H:165:THR:HG21	4:H:234:HOH:O	2.08	0.53
1:A:164:THR:HG23	1:A:165:GLU:O	2.09	0.52
2:B:151:THR:HG22	4:B:241:HOH:O	2.08	0.52
1:L:135:LEU:HD22	2:H:181:VAL:HG21	1.93	0.51
2:H:29:ILE:HG12	2:H:52(A):PRO:HG2	1.92	0.51
1:A:24:ARG:HH11	1:A:24:ARG:CG	2.25	0.50
1:A:164:THR:HG21	4:A:215:HOH:O	2.10	0.50
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.93	0.49
2:B:64:LYS:NZ	4:B:242:HOH:O	2.28	0.48
3:S:45:LYS:HB3	3:S:48:GLN:HB3	1.95	0.48
1:L:180:THR:HG23	4:L:216:HOH:O	2.13	0.48
1:L:108:ARG:HD3	1:L:109:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ARG:HD2	2:B:100(B):TRP:CZ2	2.49	0.47
2:H:22:CYS:SG	2:H:34:ILE:HD13	2.54	0.47
2:B:100(B):TRP:CA	2:B:100(C):MET:N	2.69	0.47
2:H:165:THR:HA	2:H:180:SER:HA	1.97	0.47
2:B:165:THR:HG21	4:B:250:HOH:O	2.15	0.46
1:A:189:HIS:O	1:A:211:ARG:NH1	2.49	0.46
1:L:29:VAL:CG1	1:L:92:TYR:HB2	2.46	0.46
2:B:169:VAL:HB	4:B:239:HOH:O	2.16	0.45
2:B:201:LYS:N	2:B:202:PRO:CD	2.79	0.45
1:A:166:GLN:HG2	1:A:171:SER:O	2.16	0.45
2:B:94:ARG:HG2	2:B:101:ASP:OD1	2.15	0.45
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.80	0.44
3:R:64:THR:O	3:R:82:THR:CG2	2.66	0.44
2:H:178:LEU:HD12	2:H:178:LEU:C	2.38	0.44
1:L:79:GLN:HB3	1:L:80:PRO:CD	2.48	0.44
1:A:120:PRO:HB2	1:A:125:LEU:HD13	2.00	0.43
2:H:4:LEU:HD23	2:H:24:ALA:HA	2.00	0.43
1:A:108:ARG:HD2	1:A:140:TYR:CB	2.49	0.43
2:B:165:THR:HA	2:B:180:SER:HA	2.00	0.42
1:A:186:TYR:O	1:A:192:TYR:OH	2.35	0.42
2:B:4:LEU:HD23	2:B:24:ALA:HA	2.02	0.42
2:H:22:CYS:HG	2:H:92:CYS:CB	2.31	0.42
1:A:159:SER:HA	1:A:178:THR:O	2.20	0.42
3:R:55:ASN:N	3:R:55:ASN:HD22	2.18	0.42
1:A:170:ASP:OD1	1:A:172:THR:OG1	2.32	0.42
2:H:195:ILE:HA	2:H:209:LYS:O	2.20	0.41
2:B:93:ALA:HB1	2:B:100(C):MET:HB3	2.03	0.41
2:H:100:ARG:HD2	2:H:100(B):TRP:CZ2	2.56	0.41
1:A:49:TYR:OH	3:R:53:HIS:HE1	2.03	0.40
3:R:64:THR:O	3:R:82:THR:HG23	2.22	0.40
1:L:166:GLN:HG2	1:L:171:SER:O	2.22	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	209/214 (98%)	207 (99%)	2 (1%)	0	100	100
1	L	209/214 (98%)	205 (98%)	4 (2%)	0	100	100
2	B	211/228 (92%)	204 (97%)	7 (3%)	0	100	100
2	H	211/228 (92%)	205 (97%)	5 (2%)	1 (0%)	34	40
3	R	106/130 (82%)	99 (93%)	5 (5%)	2 (2%)	10	8
3	S	62/130 (48%)	58 (94%)	3 (5%)	1 (2%)	12	10
All	All	1008/1144 (88%)	978 (97%)	26 (3%)	4 (0%)	39	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	67	ASP
3	R	67	ASP
3	R	94	GLU
2	H	32	SER

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	186/188 (99%)	175 (94%)	11 (6%)	24	32
1	L	186/188 (99%)	174 (94%)	12 (6%)	21	27
2	B	176/188 (94%)	165 (94%)	11 (6%)	22	29
2	H	176/188 (94%)	165 (94%)	11 (6%)	22	29
3	R	99/117 (85%)	93 (94%)	6 (6%)	23	30
3	S	59/117 (50%)	54 (92%)	5 (8%)	13	15
All	All	882/986 (90%)	826 (94%)	56 (6%)	22	29

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	42	LYS
1	A	108	ARG
1	A	122	ASP
1	A	125	LEU
1	A	155	GLN
1	A	164	THR
1	A	168	SER
1	A	175	LEU
1	A	180	THR
1	A	183	LYS
2	B	48	VAL
2	B	62	SER
2	B	63	VAL
2	B	94	ARG
2	B	108	LEU
2	B	135	THR
2	B	151	THR
2	B	159	LEU
2	B	165	THR
2	B	170	LEU
2	B	181	VAL
3	R	55	ASN
3	R	70	GLU
3	R	82	THR
3	R	94	GLU
3	R	101	ARG
3	R	127	HIS
1	L	1	ASP
1	L	11	LEU
1	L	56	SER
1	L	63	SER
1	L	72	THR
1	L	108	ARG
1	L	125	LEU
1	L	142	ARG
1	L	164	THR
1	L	168	SER
1	L	175	LEU
1	L	180	THR
2	H	19	ARG
2	H	63	VAL
2	H	108	LEU

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Mol	Chain	Res	Type
2	H	135	THR
2	H	151	THR
2	H	159	LEU
2	H	161	SER
2	H	165	THR
2	H	170	LEU
2	H	178	LEU
2	H	181	VAL
3	S	45	LYS
3	S	49	ASP
3	S	52	THR
3	S	67	ASP
3	S	73	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	100	GLN
1	A	198	HIS
1	A	210	ASN
3	R	53	HIS
1	L	27	GLN
1	L	198	HIS
1	L	210	ASN
3	S	53	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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 ⓘ

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	211/214 (98%)	0.56	7 (3%)	50 59	4, 14, 21, 28	0
1	L	211/214 (98%)	0.90	22 (10%)	8 13	4, 14, 21, 27	0
2	B	215/228 (94%)	0.42	7 (3%)	50 59	4, 13, 21, 39	0
2	H	215/228 (94%)	0.58	11 (5%)	32 41	4, 13, 21, 39	0
3	R	108/130 (83%)	1.98	45 (41%)	0 0	3, 12, 22, 32	8 (7%)
3	S	58/130 (44%)	3.05	34 (58%)	0 0	5, 14, 23, 27	4 (6%)
All	All	1018/1144 (88%)	0.90	126 (12%)	5 8	3, 13, 22, 39	12 (1%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	S	75	PRO	9.9
3	R	68	SER	9.5
3	R	100	CYS	9.1
3	S	76	CYS	8.9
3	S	66	CYS	8.6
3	S	29	PRO	8.2
3	R	120	TRP	7.2
2	H	128	SER	7.2
3	S	65	ARG	7.1
3	R	67	ASP	7.0
3	S	47	GLY	6.6
3	R	126	VAL	6.6
2	B	128	SER	6.5
3	S	78	THR	6.5
3	R	125	CYS	6.5
2	H	190	GLY	5.6
3	S	84	CYS	5.4
3	S	77	THR	4.9
3	R	107	CYS	4.9

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Mol	Chain	Res	Type	RSRZ
3	S	21	SER	4.8
3	S	63	CYS	4.7
2	H	96	LEU	4.5
3	S	40	ASP	4.5
3	R	71	VAL	4.4
3	S	74	SER	4.4
3	R	114	VAL	4.3
1	L	46	LEU	4.3
3	R	95	ASP	4.2
3	R	87	GLU	4.0
3	S	22	SER	4.0
1	L	48	ILE	4.0
3	R	22	SER	3.9
3	R	121	SER	3.9
3	R	119	PRO	3.9
1	L	67	SER	3.8
3	S	73	LEU	3.8
3	R	40	ASP	3.6
3	R	99	MET	3.6
3	R	21	SER	3.5
3	S	32	HIS	3.5
3	S	39	ARG	3.5
3	S	83	VAL	3.4
3	S	79	THR	3.4
1	L	47	LEU	3.4
1	L	36	TYR	3.4
3	S	61	LEU	3.3
3	S	28	CYS	3.3
1	L	92	TYR	3.2
3	R	91	PHE	3.2
2	H	1	GLU	3.1
3	R	39	ARG	3.1
3	S	82	THR	3.1
3	S	64	THR	3.0
1	L	70	ASP	3.0
3	S	57	LEU	3.0
3	R	116	ASP	2.9
3	S	27	LEU	2.9
2	B	190	GLY	2.9
2	H	134	GLY	2.9
3	R	118	THR	2.8
1	L	27	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
3	S	23	PRO	2.8
2	B	193	THR	2.8
1	L	1	ASP	2.8
1	L	156	SER	2.7
3	R	24	SER	2.7
3	R	25	GLU	2.7
3	R	123	ILE	2.6
3	R	117	CYS	2.6
3	R	66	CYS	2.6
3	S	26	GLY	2.6
3	R	96	SER	2.6
1	L	126	LYS	2.6
2	B	127	SER	2.6
1	L	34	ALA	2.6
3	R	128	LYS	2.5
1	L	184	ALA	2.5
2	B	134	GLY	2.5
3	R	73	LEU	2.5
3	S	43	SER	2.5
2	H	29	ILE	2.5
1	L	106	ILE	2.5
2	B	1	GLU	2.5
3	R	85	GLN	2.5
3	S	24	SER	2.4
3	S	48	GLN	2.4
3	R	97	PRO	2.4
3	R	110	GLY	2.4
3	S	53	HIS	2.4
3	R	23	PRO	2.4
1	L	188	LYS	2.4
1	A	122	ASP	2.4
1	A	126	LYS	2.4
2	H	100(C)	MET	2.3
3	R	69	GLY	2.3
2	B	195	ILE	2.3
1	L	16	GLY	2.3
2	H	127	SER	2.3
3	R	122	ASP	2.3
2	H	105	GLN	2.3
3	S	55	ASN	2.3
3	R	65	ARG	2.3
3	R	109	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
3	R	101	ARG	2.2
1	A	46	LEU	2.2
2	H	97	ALA	2.2
2	H	100(B)	TRP	2.2
3	S	60	CYS	2.2
1	A	184	ALA	2.2
1	A	1	ASP	2.2
1	L	81	GLU	2.1
3	R	108	PRO	2.1
1	L	24	ARG	2.1
3	S	49	ASP	2.1
1	L	29	VAL	2.1
3	R	89	GLY	2.1
1	A	8	PRO	2.1
3	R	127	HIS	2.0
1	L	73	LEU	2.0
3	R	111	MET	2.0
3	R	113	LYS	2.0
1	A	123	GLU	2.0
1	L	52	SER	2.0
1	L	65	SER	2.0
3	R	70	GLU	2.0
3	R	74	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 carbohydrates 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.