W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 27, 2023 – 02:47 AM EDT

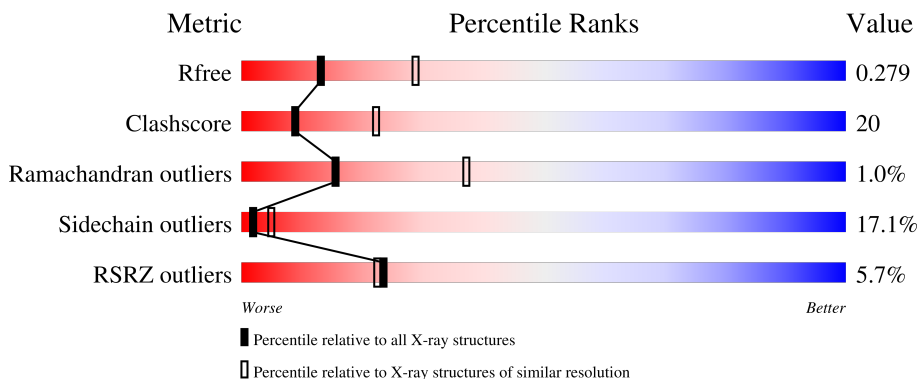|		
PDB ID	:	3NH7
Title	:	Crystal structure of the neutralizing Fab fragment AbD1556 bound to the BMP type I receptor IA
Authors	:	Mueller, T.D.; Harth, S.; Sebald, W.
Deposited on	:	2010-06-14
Resolution	:	2.70 Å(reported)

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 2.70 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.
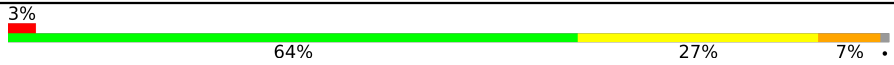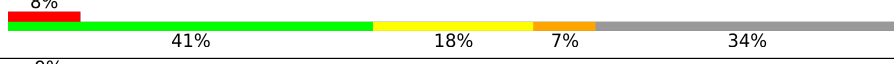
Metric	Percentile Ranks	Value
Rfree		0.279
Clashscore		20
Ramachandran outliers		1.0%
Sidechain outliers		17.1%
RSRZ outliers		5.7%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
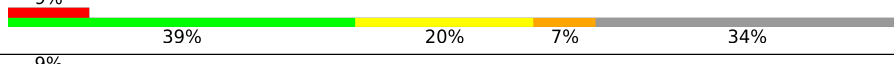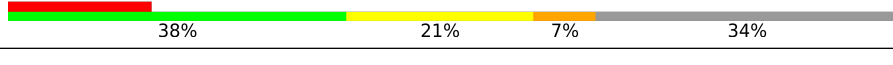
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	234	3% 47% 34% 8% 12%
1	I	234	4% 58% 26% 7% 8%
1	J	234	6% 59% 29% 6% 6%
1	K	234	3% 61% 24% 6% · 8%
2	L	213	3% 62% 30% 7% ·

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Mol	Chain	Length	Quality of chain
2	M	213	3% 64% 27% 7%
2	N	213	3% 64% 26% 8%
2	O	213	2% 62% 28% 8%
3	A	129	8% 41% 18% 7% 34%
3	B	129	9% 39% 20% 7% 34%
3	C	129	9% 40% 18% 8% 34%
3	D	129	16% 38% 21% 7% 34%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 15350 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 Antibody fragment Fab AbD1556, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	207	Total	C	N	O	S	0	0	0
			1569	992	269	303	5			
1	I	215	Total	C	N	O	S	0	0	0
			1620	1021	278	316	5			
1	J	221	Total	C	N	O	S	0	0	0
			1661	1045	286	325	5			
1	K	215	Total	C	N	O	S	0	0	0
			1625	1025	279	316	5			

- Molecule 2 is a protein called Antibody fragment Fab AbD1556, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	0	0	0
			1558	973	258	322	5			
2	M	210	Total	C	N	O	S	0	0	0
			1558	973	258	322	5			
2	N	210	Total	C	N	O	S	0	0	0
			1558	973	258	322	5			
2	O	210	Total	C	N	O	S	0	0	0
			1558	973	258	322	5			

- Molecule 3 is a protein called Bone morphogenetic protein receptor type-1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	85	Total	C	N	O	S	0	0	0
			654	400	112	131	11			
3	B	85	Total	C	N	O	S	0	0	0
			654	400	112	131	11			
3	C	85	Total	C	N	O	S	0	0	0
			654	400	112	131	11			
3	D	85	Total	C	N	O	S	0	0	0
			654	400	112	131	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	2	Total 2	O 2	0	0
4	L	3	Total 3	O 3	0	0
4	A	2	Total 2	O 2	0	0
4	I	5	Total 5	O 5	0	0
4	M	4	Total 4	O 4	0	0
4	B	1	Total 1	O 1	0	0
4	J	2	Total 2	O 2	0	0
4	N	1	Total 1	O 1	0	0
4	K	2	Total 2	O 2	0	0
4	O	4	Total 4	O 4	0	0
4	D	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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: Antibody fragment Fab AbD1556, heavy chain

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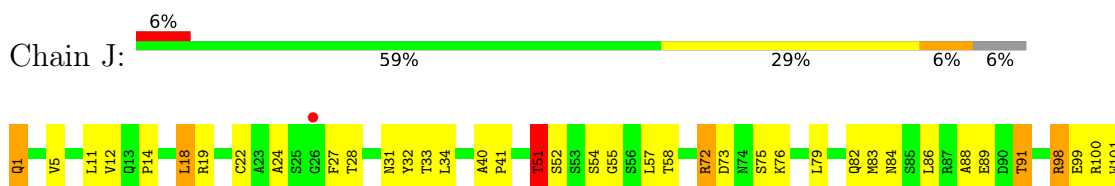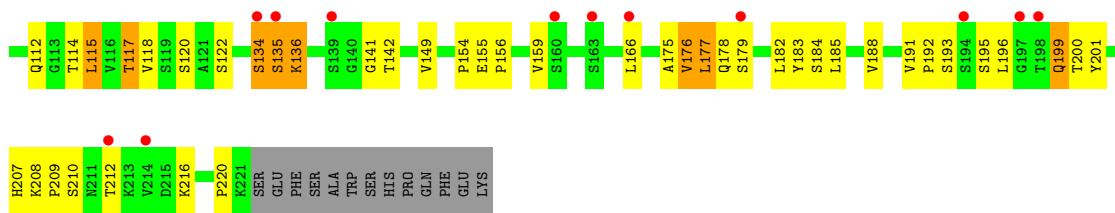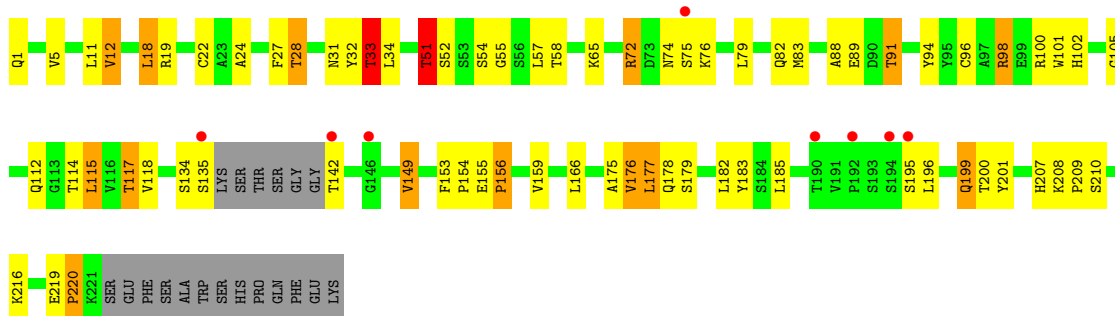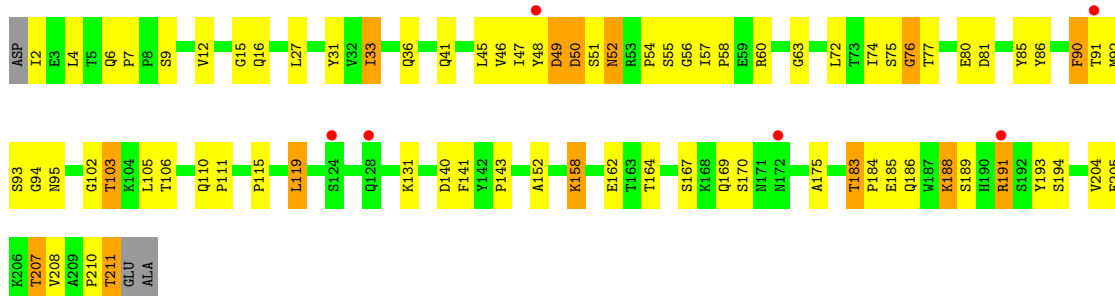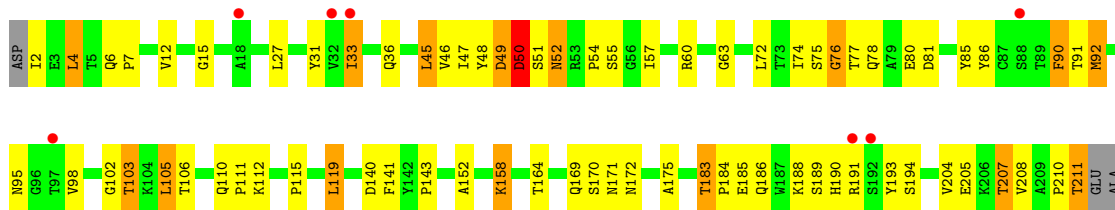Q112 G113 T114 L115 V116 T117 V118 S119 S120 A121 S122 S134 S135 K136 S139 G140 G141 T142 V149 P154 E155 P156 V159 S160 S163 L166 A175 V176 L177 Q178 S179 L182 Y183 S184 L185 V188 V191 P192 S193 S194 L196 G197 T198 Q199 T200 Y201

H207 K208 P209 S210 N211 T212 K213 V214 D215 K216 K221 P220 SER GLU PHE SER ALA TRP SER HIS PRO GLN PHE GLU LYS

• Molecule 1: Antibody fragment Fab AbD1556, heavy chain

Chain K:

3%

61% 24% 6% • 8%

Q1 V5 L11 V12 L18 R19 C22 A23 A24 F27 T28 N31 Y32 T33 L34 T51 S52 S53 S54 G55 S56 L57 T58 K65 R72 D73 N74 S75 K76 L79 Q82 M83 A88 E89 D90 T91 Y94 Y95 C96 A97 R98 E99 R100 W101 H102 G105

Q112 G113 T114 L115 V116 T117 V118 S134 S135 LYS THR SER GLY GLY T142 G146 V149 F153 P154 E155 P156 V159 L166 A175 V176 L177 Q178 S179 L182 Y183 S184 L185 T190 V191 P192 S193 S194 S195 L196 Q199 T200 Y201 H207 K208 P209 S210

K216 E219 P220 K221 SER GLU PHE SER ALA TRP SER HIS PRO GLN PHE GLU LYS

• Molecule 2: Antibody fragment Fab AbD1556, light chain

Chain L:

3%

62% 30% 7% •

ASP I2 E3 L4 T5 Q6 P7 P8 S9 V12 G15 Q16 L27 Y31 V32 I33 Q36 Q41 L45 V46 I47 Y48 D49 D50 S51 N52 R53 P54 S55 G56 I57 P58 E59 R60 G63 L72 I73 I74 S75 G76 T77 E80 D81 Y85 Y86 F90 T91 M92

S93 G94 N95 G102 T103 K104 L105 T106 Q110 P111 P115 L119 S124 Q128 K131 D140 F141 Y142 P143 A152 K158 E162 T163 T164 S167 K168 Q169 S170 N171 N172 A175 T183 P184 E185 Q186 W187 K188 S189 H190 R191 S192 Y193 S194 V204 E205

K206 T207 V208 A209 P210 T211 GLU ALA

• Molecule 2: Antibody fragment Fab AbD1556, light chain

Chain M:

3%

64% 27% 7% •

ASP I2 E3 L4 T5 Q6 P7 V12 G15 A18 L27 Y31 V32 I33 Q36 L45 V46 I47 Y48 D49 D50 S51 N52 R53 P54 S55 G56 I57 R60 G63 L72 I73 I74 S75 G76 T77 Q78 A79 E80 D81 Y85 Y86 C87 S88 T89 F90 T91 M92

N95 G96 T97 V98 G102 T103 K104 L105 T106 Q110 P111 K112 P115 L119 D140 F141 Y142 P143 A152 K158 T164 Q169 S170 N171 N172 A175 T183 P184 E185 Q186 W187 K188 S189 H190 R191 S192 Y193 S194 V204 E205 K206 T207 V208 A209 P210 T211 GLU ALA

• Molecule 2: Antibody fragment Fab AbD1556, light chain

Chain N:

3%

64% 26% 8% •

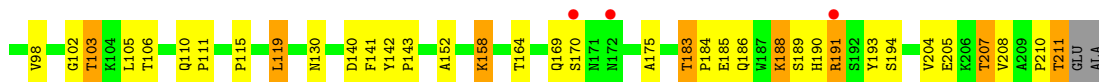• Molecule 2: Antibody fragment Fab AbD1556, light chain

Chain O:

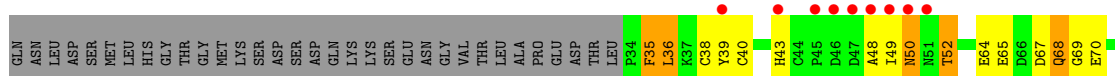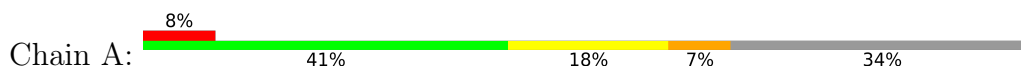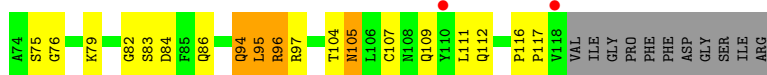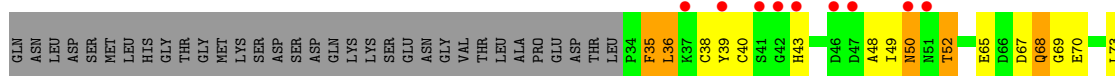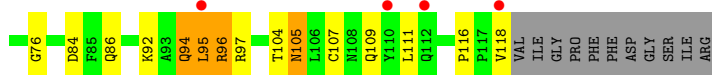• Molecule 3: Bone morphogenetic protein receptor type-1A

Chain A:

• Molecule 3: Bone morphogenetic protein receptor type-1A

Chain B:

• Molecule 3: Bone morphogenetic protein receptor type-1A

Chain C:

• Molecule 3: Bone morphogenetic protein receptor type-1A

4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.32Å 129.25Å 100.24Å 90.00° 92.27° 90.00°	Depositor
Resolution (Å)	30.40 – 2.70 30.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.3 (30.40-2.70) 95.3 (30.38-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.280 0.235 , 0.279	Depositor DCC
R_{free} test set	3020 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 61.3	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15350	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.65	0/1608	0.80	0/2190
1	I	0.65	0/1660	0.76	0/2262
1	J	0.60	0/1702	0.76	1/2318 (0.0%)
1	K	0.73	2/1665 (0.1%)	0.82	3/2268 (0.1%)
2	L	0.69	1/1595 (0.1%)	0.99	3/2180 (0.1%)
2	M	0.64	0/1595	0.80	3/2180 (0.1%)
2	N	0.69	0/1595	1.08	5/2180 (0.2%)
2	O	0.69	0/1595	0.80	3/2180 (0.1%)
3	A	0.59	0/667	0.72	0/903
3	B	0.54	0/667	0.71	0/903
3	C	0.59	1/667 (0.1%)	0.86	3/903 (0.3%)
3	D	0.53	0/667	0.72	0/903
All	All	0.65	4/15683 (0.0%)	0.84	21/21370 (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
2	L	0	1
3	A	0	1
3	B	0	1
3	C	0	1
3	D	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	191	ARG	CZ-NH2	6.19	1.41	1.33
3	C	47	ASP	CB-CG	-5.60	1.40	1.51
1	K	33	THR	CB-CG2	-5.28	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	96	CYS	CB-SG	-5.14	1.73	1.81

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	191	ARG	NE-CZ-NH1	-28.45	106.08	120.30
2	L	191	ARG	NE-CZ-NH2	23.52	132.06	120.30
2	N	191	ARG	NE-CZ-NH2	18.50	129.55	120.30
2	L	191	ARG	NE-CZ-NH1	-15.99	112.31	120.30
2	M	191	ARG	NE-CZ-NH1	-11.30	114.65	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	48	ALA	Peptide
3	B	48	ALA	Peptide
3	C	48	ALA	Peptide
3	D	48	ALA	Peptide
2	L	93	SER	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	1569	0	1526	89	0
1	I	1620	0	1576	64	0
1	J	1661	0	1623	58	0
1	K	1625	0	1586	51	0
2	L	1558	0	1507	67	0
2	M	1558	0	1507	75	0
2	N	1558	0	1507	74	0
2	O	1558	0	1507	69	0
3	A	654	0	608	38	0
3	B	654	0	608	37	0
3	C	654	0	608	37	0
3	D	654	0	608	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	1	0	0	1	0
4	D	1	0	0	0	0
4	H	2	0	0	1	0
4	I	5	0	0	1	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	3	0	0	0	0
4	M	4	0	0	2	0
4	N	1	0	0	0	0
4	O	4	0	0	0	0
All	All	15350	0	14771	610	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 20.

The worst 5 of 610 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:O:52:ASN:ND2	3:D:43:HIS:CD2	1.99	1.31
2:L:52:ASN:ND2	3:A:43:HIS:CD2	2.07	1.22
1:I:33:THR:CG2	1:I:52:SER:HA	1.70	1.20
2:O:52:ASN:ND2	3:D:43:HIS:HD2	1.37	1.18
2:M:52:ASN:ND2	3:B:43:HIS:CD2	2.12	1.17

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	201/234 (86%)	171 (85%)	24 (12%)	6 (3%)	4	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	211/234 (90%)	202 (96%)	8 (4%)	1 (0%)	29	54
1	J	219/234 (94%)	205 (94%)	13 (6%)	1 (0%)	29	54
1	K	211/234 (90%)	201 (95%)	10 (5%)	0	100	100
2	L	208/213 (98%)	199 (96%)	7 (3%)	2 (1%)	15	37
2	M	208/213 (98%)	200 (96%)	7 (3%)	1 (0%)	29	54
2	N	208/213 (98%)	202 (97%)	5 (2%)	1 (0%)	29	54
2	O	208/213 (98%)	202 (97%)	5 (2%)	1 (0%)	29	54
3	A	83/129 (64%)	74 (89%)	8 (10%)	1 (1%)	13	32
3	B	83/129 (64%)	72 (87%)	9 (11%)	2 (2%)	6	15
3	C	83/129 (64%)	74 (89%)	7 (8%)	2 (2%)	6	15
3	D	83/129 (64%)	74 (89%)	7 (8%)	2 (2%)	6	15
All	All	2006/2304 (87%)	1876 (94%)	110 (6%)	20 (1%)	15	37

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	123	THR
1	H	192	PRO
2	L	76	GLY
2	L	94	GLY
2	M	76	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	175/198 (88%)	145 (83%)	30 (17%)	2	5
1	I	181/198 (91%)	150 (83%)	31 (17%)	2	5
1	J	186/198 (94%)	151 (81%)	35 (19%)	1	4
1	K	182/198 (92%)	148 (81%)	34 (19%)	1	4
2	L	176/178 (99%)	148 (84%)	28 (16%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
2	M	176/178 (99%)	152 (86%)	24 (14%)	3	8	
2	N	176/178 (99%)	151 (86%)	25 (14%)	3	8	
2	O	176/178 (99%)	149 (85%)	27 (15%)	2	7	
3	A	76/114 (67%)	62 (82%)	14 (18%)	1	4	
3	B	76/114 (67%)	59 (78%)	17 (22%)	1	2	
3	C	76/114 (67%)	61 (80%)	15 (20%)	1	3	
3	D	76/114 (67%)	60 (79%)	16 (21%)	1	3	
All	All	1732/1960 (88%)	1436 (83%)	296 (17%)	2	5	

5 of 296 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	65	LYS
3	D	68	GLN
1	K	134	SER
2	O	50	ASP
1	I	184	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	37	GLN
2	O	65	ASN
3	D	86	GLN
1	I	162	ASN
1	I	84	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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(Å²)	Q<0.9
1	H	207/234 (88%)	0.01	8 (3%)	39	38	37, 54, 91, 122	0
1	I	215/234 (91%)	0.25	10 (4%)	31	30	38, 56, 89, 114	0
1	J	221/234 (94%)	0.41	13 (5%)	22	21	44, 64, 102, 125	0
1	K	215/234 (91%)	0.19	8 (3%)	41	41	37, 54, 95, 123	0
2	L	210/213 (98%)	0.29	6 (2%)	51	52	44, 61, 86, 112	0
2	M	210/213 (98%)	0.31	7 (3%)	46	46	41, 59, 77, 92	0
2	N	210/213 (98%)	0.19	7 (3%)	46	46	48, 59, 78, 93	0
2	O	210/213 (98%)	0.06	4 (1%)	66	69	44, 57, 72, 86	0
3	A	85/129 (65%)	0.71	10 (11%)	4	3	51, 73, 107, 127	0
3	B	85/129 (65%)	0.78	11 (12%)	3	2	52, 79, 112, 135	0
3	C	85/129 (65%)	0.83	12 (14%)	2	1	58, 78, 108, 127	0
3	D	85/129 (65%)	1.07	20 (23%)	0	0	50, 80, 131, 157	0
All	All	2038/2304 (88%)	0.32	116 (5%)	23	22	37, 61, 99, 157	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	46	ASP	7.4
3	B	118	VAL	7.1
3	B	42	GLY	6.7
3	D	48	ALA	6.0
3	C	34	PRO	5.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.