Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 07:56 AM EDT

PDB ID	:	3SKJ
Title	:	Structural And Functional Characterization of an Agonistic Anti-Human EphA2 Monoclonal Antibody
Authors	:	Oganesyan, V.Y.; Wu, H.; Dall'Acqua, W.F.
Deposited on	:	2011-06-22
Resolution	:	2.50 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:

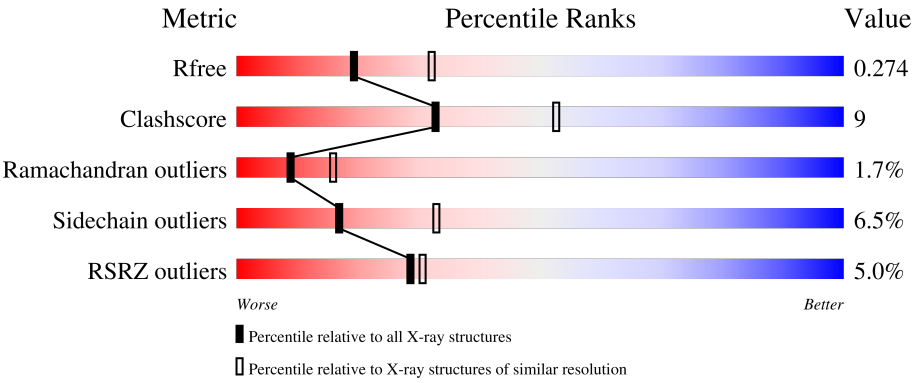
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	L	214	3% 76% 20% ·
1	M	214	5% 76% 21% ·
2	H	231	% 73% 22% · ·
2	I	231	4% 73% 23% · ·
3	E	206	% 72% 13% 15%

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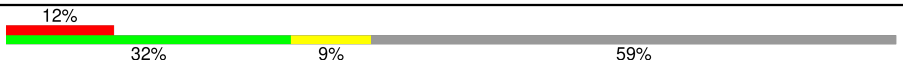
Mol	Chain	Length	Quality of chain
3	F	206	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8819 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, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1651	1031	280	334	6			
1	M	214	Total	C	N	O	S	0	0	0
			1651	1031	280	334	6			

- Molecule 2 is a protein called Antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	228	Total	C	N	O	S	0	1	0
			1704	1076	290	330	8			
2	I	228	Total	C	N	O	S	0	0	0
			1696	1069	287	332	8			

- Molecule 3 is a protein called Ephrin type-A receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	176	Total	C	N	O	S	0	0	0
			1415	906	235	265	9			
3	F	84	Total	C	N	O	S	0	0	0
			659	413	109	128	9			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-27	ALA	-	expression tag	UNP P29317
E	-26	PRO	-	expression tag	UNP P29317
E	-25	GLU	-	expression tag	UNP P29317
E	-24	HIS	-	expression tag	UNP P29317
E	-23	HIS	-	expression tag	UNP P29317
E	-22	HIS	-	expression tag	UNP P29317
E	-21	HIS	-	expression tag	UNP P29317
E	-20	HIS	-	expression tag	UNP P29317

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	HIS	-	expression tag	UNP P29317
E	-18	ASP	-	expression tag	UNP P29317
E	-17	TYR	-	expression tag	UNP P29317
E	-16	ASP	-	expression tag	UNP P29317
E	-15	ILE	-	expression tag	UNP P29317
E	-14	PRO	-	expression tag	UNP P29317
E	-13	THR	-	expression tag	UNP P29317
E	-12	THR	-	expression tag	UNP P29317
E	-11	GLU	-	expression tag	UNP P29317
E	-10	ASN	-	expression tag	UNP P29317
E	-9	LEU	-	expression tag	UNP P29317
E	-8	TYR	-	expression tag	UNP P29317
E	-7	PHE	-	expression tag	UNP P29317
E	-6	GLN	-	expression tag	UNP P29317
E	-5	GLY	-	expression tag	UNP P29317
E	-4	ALA	-	expression tag	UNP P29317
E	-3	MET	-	expression tag	UNP P29317
E	-2	ASP	-	expression tag	UNP P29317
F	-27	ALA	-	expression tag	UNP P29317
F	-26	PRO	-	expression tag	UNP P29317
F	-25	GLU	-	expression tag	UNP P29317
F	-24	HIS	-	expression tag	UNP P29317
F	-23	HIS	-	expression tag	UNP P29317
F	-22	HIS	-	expression tag	UNP P29317
F	-21	HIS	-	expression tag	UNP P29317
F	-20	HIS	-	expression tag	UNP P29317
F	-19	HIS	-	expression tag	UNP P29317
F	-18	ASP	-	expression tag	UNP P29317
F	-17	TYR	-	expression tag	UNP P29317
F	-16	ASP	-	expression tag	UNP P29317
F	-15	ILE	-	expression tag	UNP P29317
F	-14	PRO	-	expression tag	UNP P29317
F	-13	THR	-	expression tag	UNP P29317
F	-12	THR	-	expression tag	UNP P29317
F	-11	GLU	-	expression tag	UNP P29317
F	-10	ASN	-	expression tag	UNP P29317
F	-9	LEU	-	expression tag	UNP P29317
F	-8	TYR	-	expression tag	UNP P29317
F	-7	PHE	-	expression tag	UNP P29317
F	-6	GLN	-	expression tag	UNP P29317
F	-5	GLY	-	expression tag	UNP P29317
F	-4	ALA	-	expression tag	UNP P29317

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	MET	-	expression tag	UNP P29317
F	-2	ASP	-	expression tag	UNP P29317

- Molecule 4 is water.

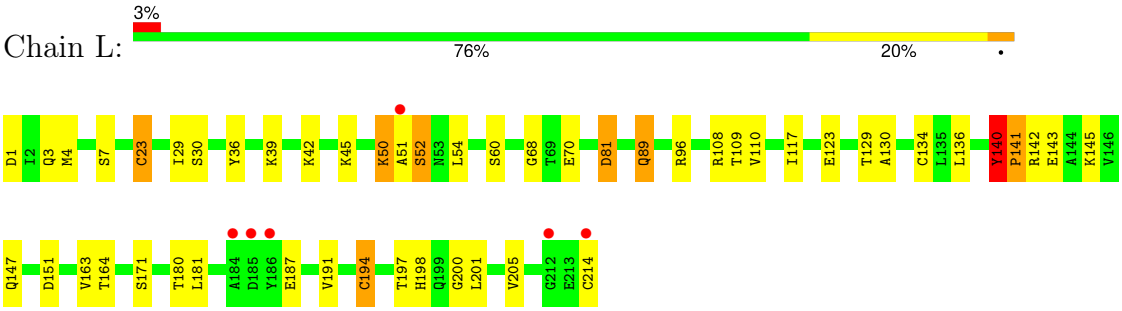
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	7	Total O 7 7	0	0
4	H	13	Total O 13 13	0	0
4	M	6	Total O 6 6	0	0
4	I	8	Total O 8 8	0	0
4	E	9	Total O 9 9	0	0

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.

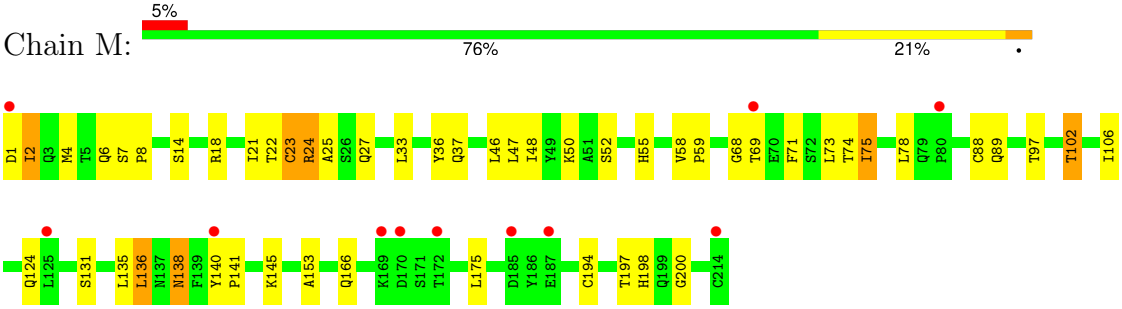
• Molecule 1: Antibody, light chain

Chain L:



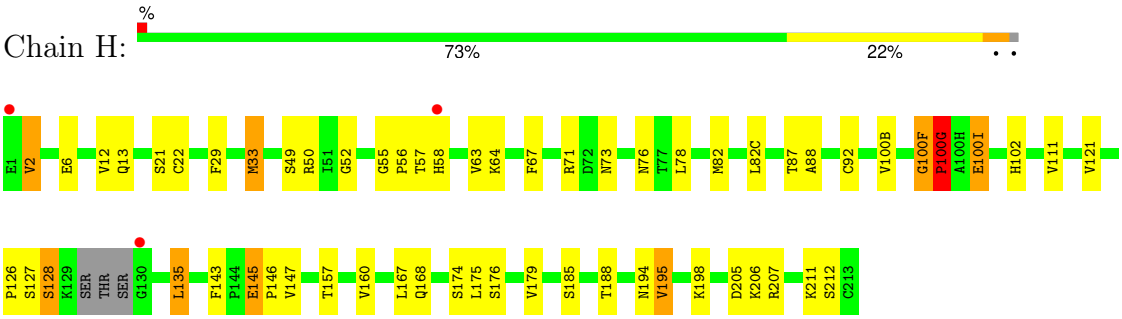
• Molecule 1: Antibody, light chain

Chain M:



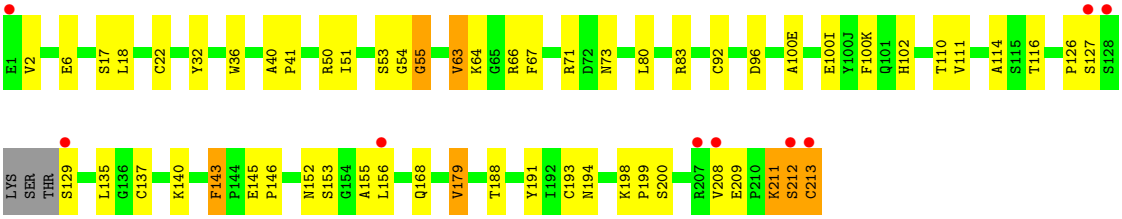
• Molecule 2: Antibody, heavy chain

Chain H:

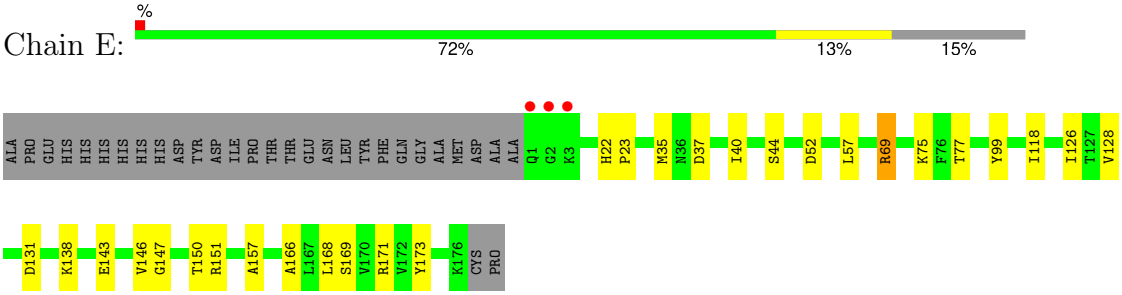


• Molecule 2: Antibody, heavy chain

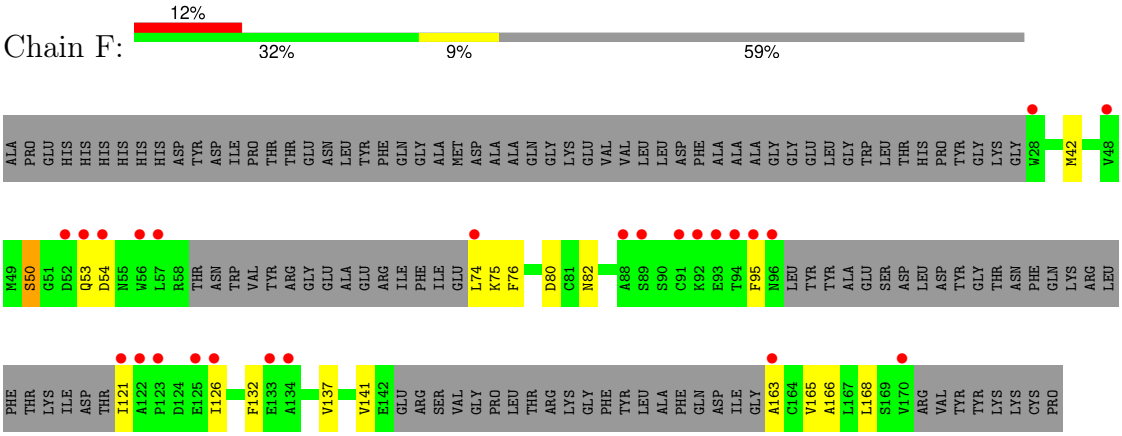
Chain I:



• Molecule 3: Ephrin type-A receptor 2



• Molecule 3: Ephrin type-A receptor 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	78.94Å 120.86Å 286.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 35.88 – 2.48	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-2.50) 94.4 (35.88-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.271 0.221 , 0.274	Depositor DCC
R_{free} test set	2278 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8819	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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	L	0.80	2/1687 (0.1%)	0.81	1/2287 (0.0%)
1	M	0.69	1/1687 (0.1%)	0.78	1/2287 (0.0%)
2	H	0.92	3/1753 (0.2%)	0.88	4/2387 (0.2%)
2	I	0.77	2/1740 (0.1%)	0.80	2/2369 (0.1%)
3	E	0.80	0/1449	0.81	0/1960
3	F	0.67	0/669	0.76	0/902
All	All	0.79	8/8985 (0.1%)	0.81	8/12192 (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
1	L	0	3
1	M	0	2
2	H	0	4
2	I	0	5
3	E	0	1
All	All	0	15

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	100(G)	PRO	N-CD	18.12	1.73	1.47
2	I	213	CYS	C-OXT	7.88	1.38	1.23
1	L	23	CYS	CB-SG	-6.39	1.71	1.82
1	L	194	CYS	CB-SG	-6.29	1.71	1.82
2	H	92	CYS	CB-SG	-5.57	1.72	1.81
2	I	137	CYS	CB-SG	-5.49	1.72	1.81
2	H	100(F)	GLY	C-N	-5.20	1.24	1.34
1	M	23	CYS	CB-SG	-5.05	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	24	ARG	NE-CZ-NH1	8.01	124.30	120.30
2	H	100(G)	PRO	N-CA-CB	7.77	112.62	103.30
2	H	135	LEU	CA-CB-CG	6.79	130.92	115.30
1	L	81	ASP	CB-CG-OD1	-6.02	112.88	118.30
2	H	100(G)	PRO	CA-N-CD	-5.27	104.12	111.50
2	I	83	ARG	NE-CZ-NH1	5.23	122.91	120.30
2	I	66	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	H	207	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	22	HIS	Peptide
2	H	143	PHE	Mainchain,Peptide
2	H	145	GLU	Mainchain,Peptide
2	I	143	PHE	Mainchain,Peptide
2	I	145	GLU	Mainchain,Peptide
2	I	53	SER	Peptide
1	L	140	TYR	Peptide
1	L	7	SER	Mainchain,Peptide
1	M	140	TYR	Peptide
1	M	7	SER	Peptide

5.2 Too-close contacts (i)

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	L	1651	0	1604	28	0
1	M	1651	0	1605	33	0
2	H	1704	0	1648	36	0
2	I	1696	0	1639	34	0
3	E	1415	0	1367	13	0
3	F	659	0	624	10	0
4	E	9	0	0	2	0
4	H	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	8	0	0	0	0
4	L	7	0	0	0	0
4	M	6	0	0	0	0
All	All	8819	0	8487	147	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 9.

All (147) 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:H:100(G):PRO:N	2:H:100(G):PRO:CD	1.73	1.39
2:I:212:SER:O	2:I:213:CYS:SG	1.95	1.25
2:H:121:VAL:HG21	2:H:195:VAL:HG11	1.30	1.10
2:I:2:VAL:HG11	2:I:102:HIS:ND1	1.75	1.01
1:M:23:CYS:HG	1:M:88:CYS:HG	0.93	0.89
1:L:51:ALA:O	1:L:52:SER:HB3	1.76	0.84
2:I:71:ARG:HE	2:I:73:ASN:HD21	1.26	0.83
2:H:160:VAL:HG22	2:H:179:VAL:CG1	2.11	0.80
2:H:100(F):GLY:C	2:H:100(G):PRO:CD	2.51	0.78
2:H:50:ARG:NH2	2:H:56:PRO:HG2	2.02	0.73
2:H:71:ARG:HE	2:H:73:ASN:HD21	1.34	0.73
2:H:2:VAL:HG11	2:H:102:HIS:CE1	2.23	0.72
2:I:126:PRO:HD3	2:I:135:LEU:HD23	1.71	0.71
2:I:156:LEU:HD21	2:I:179:VAL:HG11	1.73	0.71
1:L:140:TYR:CD2	1:L:141:PRO:HD3	2.26	0.70
2:H:33:MET:SD	2:H:50:ARG:NH1	2.66	0.69
2:I:153:SER:H	2:I:194:ASN:HD21	1.39	0.69
3:E:128:VAL:HG22	3:E:131:ASP:OD1	1.93	0.67
2:I:22:CYS:HG	2:I:92:CYS:HG	1.20	0.66
1:M:4:MET:HE2	1:M:25:ALA:HA	1.78	0.64
1:L:180:THR:O	1:L:181:LEU:HD23	1.98	0.63
2:I:212:SER:C	2:I:213:CYS:SG	2.78	0.62
1:M:2:ILE:HG12	1:M:27:GLN:HE21	1.65	0.62
2:H:52:GLY:HA3	2:H:56:PRO:HD2	1.82	0.60
1:M:48:ILE:CD1	1:M:73:LEU:HD13	2.32	0.59
2:H:71:ARG:HE	2:H:73:ASN:ND2	2.01	0.58
1:L:109:THR:HG22	1:L:110:VAL:O	2.04	0.58
1:L:143:GLU:HG2	1:M:153:ALA:HB2	1.86	0.57
2:I:211:LYS:O	2:I:213:CYS:OXT	2.23	0.57
1:L:129:THR:HG22	1:L:130:ALA:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:69:ARG:NH1	3:E:147:GLY:HA2	2.20	0.57
1:M:6:GLN:NE2	1:M:102:THR:HG22	2.20	0.56
2:H:160:VAL:HG22	2:H:179:VAL:HG12	1.86	0.56
1:M:75:ILE:HD11	1:M:78:LEU:HA	1.88	0.56
2:H:168:GLN:NE2	2:H:174:SER:HB2	2.21	0.55
3:E:35:MET:HB2	3:E:40:ILE:HD12	1.89	0.55
2:I:71:ARG:NE	2:I:73:ASN:HD21	2.01	0.55
2:I:116:THR:HG22	2:I:200:SER:HB3	1.89	0.55
2:I:135:LEU:HD22	2:I:208:VAL:CG1	2.37	0.55
2:I:17:SER:O	2:I:18:LEU:HD23	2.06	0.55
2:H:185:SER:O	2:H:188:THR:HG22	2.07	0.54
2:I:211:LYS:O	2:I:212:SER:C	2.46	0.54
1:L:151:ASP:HA	1:L:191:VAL:CG1	2.38	0.54
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.89	0.54
1:M:6:GLN:HE21	1:M:102:THR:HG22	1.73	0.54
3:E:75:LYS:NZ	4:E:181:HOH:O	2.40	0.54
2:H:168:GLN:HE21	2:H:174:SER:HB2	1.72	0.53
2:H:50:ARG:HH22	2:H:56:PRO:HG2	1.72	0.53
1:M:37:GLN:HB2	1:M:47:LEU:HD11	1.90	0.53
2:H:71:ARG:NE	2:H:73:ASN:HD21	2.05	0.53
2:I:211:LYS:O	2:I:213:CYS:N	2.41	0.53
2:H:87:THR:O	2:H:88:ALA:HB2	2.08	0.53
2:I:36:TRP:CD1	2:I:80:LEU:HD13	2.43	0.53
2:I:54:GLY:O	2:I:55:GLY:O	2.27	0.52
1:L:214:CYS:HA	2:H:211:LYS:HE3	1.90	0.52
1:M:21:ILE:HD12	1:M:102:THR:CG2	2.40	0.52
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.91	0.52
1:L:142:ARG:NE	1:L:163:VAL:HG21	2.25	0.51
3:F:137:VAL:HG23	3:F:137:VAL:O	2.11	0.51
1:M:50:LYS:O	1:M:50:LYS:HG2	2.10	0.51
1:L:117:ILE:HD12	1:L:194:CYS:HB2	1.92	0.51
1:L:140:TYR:O	1:L:141:PRO:O	2.29	0.51
3:E:75:LYS:HB2	3:E:169:SER:HB3	1.93	0.50
2:I:140:LYS:NZ	2:I:168:GLN:HE22	2.10	0.50
1:L:50:LYS:O	1:L:51:ALA:HB3	2.10	0.50
2:I:2:VAL:HG11	2:I:102:HIS:CG	2.46	0.49
1:L:151:ASP:HA	1:L:191:VAL:HG13	1.94	0.49
1:M:22:THR:HG22	1:M:23:CYS:N	2.28	0.49
1:M:136:LEU:HD23	1:M:136:LEU:N	2.28	0.49
1:M:135:LEU:C	1:M:136:LEU:HD23	2.34	0.48
2:H:121:VAL:CG2	2:H:195:VAL:HG11	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:18:ARG:NH1	1:M:74:THR:HG21	2.28	0.48
3:E:75:LYS:NZ	4:E:180:HOH:O	2.45	0.48
2:I:63:VAL:HG13	2:I:67:PHE:HB2	1.96	0.48
3:F:75:LYS:HG2	3:F:141:VAL:HG22	1.95	0.48
1:M:33:LEU:HD22	1:M:71:PHE:CG	2.49	0.47
2:I:135:LEU:HD22	2:I:208:VAL:HG12	1.95	0.47
2:H:57:THR:O	2:H:58[B]:HIS:HD2	1.96	0.47
1:M:4:MET:CE	1:M:25:ALA:CB	2.93	0.47
2:I:100(E):ALA:HB2	3:F:132:PHE:CZ	2.49	0.47
3:E:150:THR:HG22	3:E:151:ARG:NH2	2.29	0.47
2:I:153:SER:H	2:I:194:ASN:ND2	2.10	0.47
3:E:143:GLU:OE2	3:E:173:TYR:OH	2.26	0.47
1:L:36:TYR:OH	1:L:89:GLN:NE2	2.48	0.47
1:L:140:TYR:O	1:L:198:HIS:HE1	1.96	0.47
1:L:54:LEU:HD21	1:L:60:SER:HA	1.97	0.47
2:H:100(F):GLY:CA	2:H:100(G):PRO:CD	2.92	0.47
2:H:6:GLU:HA	2:H:21:SER:O	2.15	0.46
1:M:46:LEU:HD23	1:M:55:HIS:CG	2.50	0.46
3:F:95:PHE:CE1	3:F:121:ILE:HD12	2.51	0.46
3:E:77:THR:HG22	3:E:138:LYS:O	2.14	0.46
2:H:121:VAL:HG21	2:H:195:VAL:CG1	2.22	0.46
1:M:106:ILE:H	1:M:166:GLN:HE22	1.64	0.45
1:M:175:LEU:C	1:M:175:LEU:HD23	2.37	0.45
1:L:50:LYS:HG3	2:H:100(B):VAL:HG12	1.99	0.45
1:M:48:ILE:HD12	1:M:73:LEU:HD13	1.97	0.45
2:I:51:ILE:O	2:I:51:ILE:HG23	2.17	0.45
1:L:29:ILE:O	1:L:30:SER:C	2.56	0.45
2:H:121:VAL:O	2:H:206:LYS:HE3	2.17	0.45
3:F:42:MET:CB	3:F:168:LEU:HD23	2.46	0.45
2:I:152:ASN:O	2:I:155:ALA:HB3	2.16	0.45
3:F:163:ALA:O	3:F:165:VAL:HG23	2.17	0.44
1:L:96:ARG:NH1	2:H:100(I):GLU:OE1	2.50	0.44
1:M:33:LEU:HD11	1:M:88:CYS:HB2	1.99	0.44
3:F:42:MET:HB3	3:F:168:LEU:HD23	2.00	0.44
1:M:124:GLN:HE22	1:M:131:SER:HB2	1.82	0.44
1:M:198:HIS:CD2	1:M:200:GLY:H	2.35	0.44
2:H:29:PHE:HB3	2:H:76:ASN:ND2	2.33	0.44
2:H:194:ASN:ND2	2:H:205:ASP:OD1	2.49	0.44
2:H:160:VAL:HA	2:H:179:VAL:HG12	2.00	0.44
1:L:163:VAL:HG12	1:L:164:THR:O	2.18	0.43
1:M:21:ILE:HD12	1:M:102:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:57:LEU:O	3:E:157:ALA:HA	2.17	0.43
3:E:150:THR:CG2	3:E:151:ARG:NH2	2.81	0.43
2:H:127:SER:O	2:H:128:SER:HB3	2.18	0.43
3:F:76:PHE:HB2	3:F:166:ALA:O	2.19	0.43
2:I:100(I):GLU:OE1	2:I:100(I):GLU:N	2.51	0.43
1:L:145:LYS:HB3	1:L:197:THR:HB	2.00	0.43
1:M:145:LYS:HB3	1:M:197:THR:HB	2.01	0.43
1:L:39:LYS:HB2	1:L:42:LYS:HD2	2.00	0.42
1:M:36:TYR:HH	2:I:100(K):PHE:HD2	1.67	0.42
2:I:135:LEU:HD11	2:I:191:TYR:CD2	2.54	0.42
2:H:64:LYS:HE3	2:H:64:LYS:HB2	1.80	0.42
1:M:124:GLN:HE22	1:M:131:SER:CB	2.32	0.42
3:E:77:THR:OG1	3:E:166:ALA:HB3	2.20	0.42
2:I:156:LEU:CD2	2:I:179:VAL:HG11	2.47	0.42
1:M:58:VAL:HG13	1:M:59:PRO:HD2	2.01	0.42
1:L:108:ARG:HG3	1:L:171:SER:HB2	2.01	0.42
2:I:40:ALA:HB1	2:I:41:PRO:HD2	2.01	0.42
2:I:198:LYS:N	2:I:199:PRO:CD	2.82	0.42
3:F:50:SER:HB2	3:F:53:GLN:HE21	1.85	0.42
1:M:4:MET:HE1	1:M:25:ALA:CB	2.50	0.41
3:F:80:ASP:HB2	3:F:126:ILE:HD12	2.00	0.41
1:M:106:ILE:H	1:M:166:GLN:NE2	2.18	0.41
1:L:123:GLU:OE1	2:H:206:LYS:NZ	2.50	0.41
1:L:180:THR:C	1:L:181:LEU:HD23	2.41	0.41
1:M:48:ILE:CD1	1:M:73:LEU:CD1	2.98	0.41
1:L:198:HIS:CD2	1:L:200:GLY:H	2.38	0.41
2:I:114:ALA:HB3	2:I:143:PHE:CE1	2.55	0.41
2:H:22:CYS:HB3	2:H:78:LEU:HB3	2.03	0.40
1:L:4:MET:HE3	1:L:23:CYS:SG	2.60	0.40
3:E:118:ILE:HG12	3:E:146:VAL:HG11	2.03	0.40
2:I:22:CYS:HG	2:I:92:CYS:CB	2.34	0.40
2:I:32:TYR:CE1	2:I:96:ASP:HB2	2.56	0.40
2:H:33:MET:HE2	2:H:33:MET:HB2	1.97	0.40
1:L:201:LEU:HD22	1:L:205:VAL:HG21	2.02	0.40
1:M:138:ASN:HD22	1:M:138:ASN:N	2.19	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	L	212/214 (99%)	200 (94%)	8 (4%)	4 (2%)	8 13
1	M	212/214 (99%)	197 (93%)	10 (5%)	5 (2%)	6 9
2	H	225/231 (97%)	213 (95%)	7 (3%)	5 (2%)	6 10
2	I	224/231 (97%)	210 (94%)	11 (5%)	3 (1%)	12 21
3	E	174/206 (84%)	168 (97%)	5 (3%)	1 (1%)	25 43
3	F	76/206 (37%)	67 (88%)	8 (10%)	1 (1%)	12 21
All	All	1123/1302 (86%)	1055 (94%)	49 (4%)	19 (2%)	9 16

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	52	SER
1	L	141	PRO
2	H	128	SER
1	L	68	GLY
1	L	140	TYR
2	H	55	GLY
2	I	55	GLY
2	I	127	SER
2	H	100(G)	PRO
1	M	8	PRO
1	M	52	SER
2	I	212	SER
3	E	23	PRO
2	H	145	GLU
1	M	141	PRO
3	F	50	SER
1	M	2	ILE
2	H	126	PRO
1	M	68	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	L	188/188 (100%)	177 (94%)	11 (6%)	19	37
1	M	188/188 (100%)	177 (94%)	11 (6%)	19	37
2	H	187/189 (99%)	170 (91%)	17 (9%)	9	18
2	I	186/189 (98%)	173 (93%)	13 (7%)	15	29
3	E	151/176 (86%)	143 (95%)	8 (5%)	22	43
3	F	76/176 (43%)	73 (96%)	3 (4%)	32	57
All	All	976/1106 (88%)	913 (94%)	63 (6%)	17	33

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	3	GLN
1	L	45	LYS
1	L	50	LYS
1	L	70	GLU
1	L	81	ASP
1	L	89	GLN
1	L	134	CYS
1	L	136	LEU
1	L	147	GLN
1	L	187	GLU
2	H	2	VAL
2	H	12	VAL
2	H	13	GLN
2	H	33	MET
2	H	49	SER
2	H	100(I)	GLU
2	H	111	VAL
2	H	135	LEU
2	H	146	PRO
2	H	147	VAL
2	H	157	THR

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Mol	Chain	Res	Type
2	H	167	LEU
2	H	175	LEU
2	H	176	SER
2	H	195	VAL
2	H	198	LYS
2	H	212	SER
1	M	1	ASP
1	M	14	SER
1	M	24	ARG
1	M	69	THR
1	M	75	ILE
1	M	89	GLN
1	M	97	THR
1	M	102	THR
1	M	136	LEU
1	M	138	ASN
1	M	194	CYS
2	I	6	GLU
2	I	50	ARG
2	I	63	VAL
2	I	64	LYS
2	I	110	THR
2	I	111	VAL
2	I	129	SER
2	I	146	PRO
2	I	179	VAL
2	I	188	THR
2	I	193	CYS
2	I	209	GLU
2	I	211	LYS
3	E	37	ASP
3	E	44	SER
3	E	52	ASP
3	E	69	ARG
3	E	99	TYR
3	E	126	ILE
3	E	168	LEU
3	E	171	ARG
3	F	54	ASP
3	F	74	LEU
3	F	82	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33)

such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	79	GLN
1	L	89	GLN
1	L	198	HIS
1	L	210	ASN
2	H	39	GLN
2	H	73	ASN
2	H	76	ASN
2	H	102	HIS
2	H	105	GLN
2	H	168	GLN
1	M	27	GLN
1	M	38	GLN
1	M	79	GLN
1	M	89	GLN
1	M	137	ASN
1	M	138	ASN
1	M	166	GLN
1	M	198	HIS
2	I	39	GLN
2	I	73	ASN
2	I	76	ASN
2	I	161	HIS
2	I	168	GLN
2	I	194	ASN
2	I	196	ASN
3	E	47	ASN
3	E	82	ASN
3	E	109	ASN
3	F	32	GLN
3	F	47	ASN
3	F	53	GLN
3	F	55	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 (i)

There are no monosaccharides 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 (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, 95^{th} 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	L	214/214 (100%)	0.21	6 (2%) 53 56	32, 51, 84, 99	0
1	M	214/214 (100%)	0.38	11 (5%) 28 29	39, 62, 84, 117	0
2	H	228/231 (98%)	0.10	3 (1%) 77 79	31, 46, 59, 82	1 (0%)
2	I	228/231 (98%)	0.20	9 (3%) 39 42	37, 51, 84, 147	0
3	E	176/206 (85%)	0.13	3 (1%) 70 72	30, 48, 70, 113	0
3	F	84/206 (40%)	1.26	25 (29%) 0 0	42, 72, 104, 158	0
All	All	1144/1302 (87%)	0.28	57 (4%) 28 30	30, 52, 84, 158	1 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	213	CYS	8.3
3	E	2	GLY	7.3
1	L	214	CYS	6.5
1	M	214	CYS	5.7
1	L	184	ALA	5.3
3	F	56	TRP	4.8
3	F	95	PHE	4.4
3	F	91	CYS	4.4
3	F	122	ALA	4.3
1	M	125	LEU	4.2
2	I	129	SER	4.0
1	M	187	GLU	3.8
2	H	130	GLY	3.8
3	F	52	ASP	3.7
3	F	88	ALA	3.5
3	F	28	TRP	3.5
2	I	128	SER	3.4
2	I	207	ARG	3.3
3	F	54	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	M	170	ASP	3.3
3	F	94	THR	3.2
3	F	48	VAL	3.1
3	F	53	GLN	3.0
2	I	127	SER	2.9
3	E	1	GLN	2.9
3	F	163	ALA	2.9
3	F	96	ASN	2.9
1	L	186	TYR	2.8
2	I	212	SER	2.7
3	F	89	SER	2.7
3	F	133	GLU	2.7
3	F	92	LYS	2.7
3	F	123	PRO	2.7
3	F	121	ILE	2.5
3	F	57	LEU	2.5
1	M	69	THR	2.5
1	M	1	ASP	2.4
3	F	74	LEU	2.4
2	I	156	LEU	2.3
2	H	58[A]	HIS	2.3
2	H	1	GLU	2.3
2	I	208	VAL	2.3
3	F	126	ILE	2.3
3	F	125	GLU	2.3
3	F	93	GLU	2.2
1	L	212	GLY	2.2
3	F	170	VAL	2.2
1	M	172	THR	2.2
1	L	185	ASP	2.2
1	M	140	TYR	2.2
1	M	169	LYS	2.1
1	M	185	ASP	2.1
3	F	134	ALA	2.1
2	I	1	GLU	2.1
1	L	51	ALA	2.1
1	M	80	PRO	2.1
3	E	3	LYS	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 monosaccharides 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.