Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2024 – 04:10 PM EST

PDB ID	:	8SI1
Title	:	Ara h 6 16A8 complex
Authors	:	Spiller, B.W.; Shrem, R.A.
Deposited on	:	2023-04-14
Resolution	:	3.20 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:

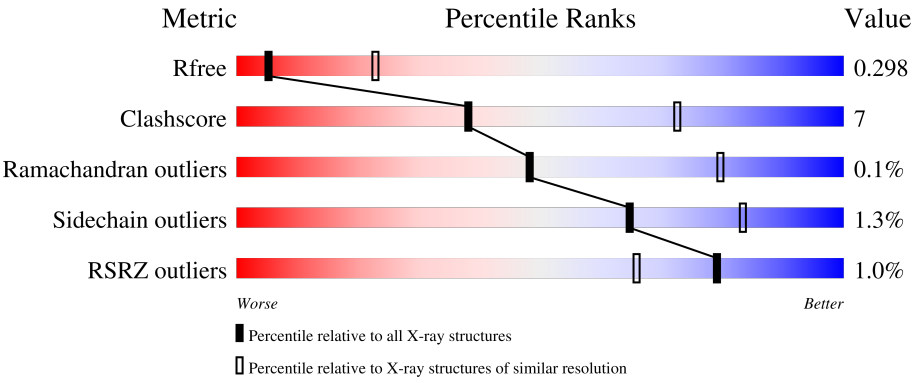
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.20 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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	A	215	% 82% 15% .
1	C	215	79% 17% 5%
1	L	215	% 77% 19% .
2	B	224	75% 20% .
2	D	224	76% 17% 7%

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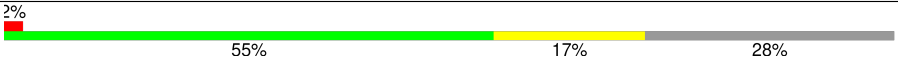
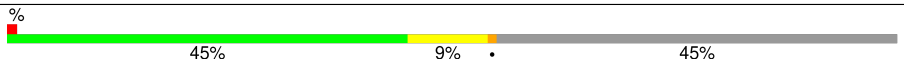
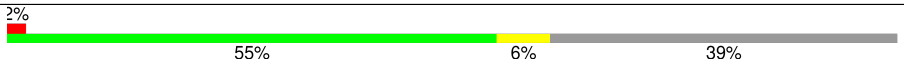
Mol	Chain	Length	Quality of chain
2	H	224	
3	E	122	
3	F	122	
3	G	122	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11439 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 16A8 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	206	Total	C	N	O	S	0	0	0
			1571	981	269	316	5			
1	A	208	Total	C	N	O	S	0	0	0
			1596	996	274	321	5			
1	C	205	Total	C	N	O	S	0	0	0
			1567	976	268	318	5			

- Molecule 2 is a protein called 16A8 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1646	1039	272	329	6			
2	B	214	Total	C	N	O	S	0	0	0
			1616	1021	266	323	6			
2	D	209	Total	C	N	O	S	0	0	0
			1576	997	259	314	6			

- Molecule 3 is a protein called Conglutin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	88	Total	C	N	O	S	0	0	0
			714	422	139	138	15			
3	G	74	Total	C	N	O	S	0	0	0
			607	362	117	115	13			
3	F	67	Total	C	N	O	S	0	0	0
			546	325	104	104	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	initiating methionine	UNP Q647G9
E	59	GLY	ARG	conflict	UNP Q647G9

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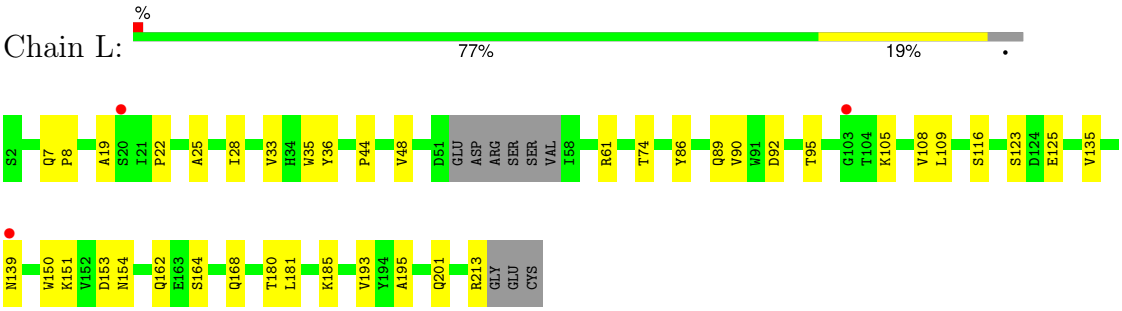
Chain	Residue	Modelled	Actual	Comment	Reference
E	91	SER	ASN	conflict	UNP Q647G9
E	114	SER	-	expression tag	UNP Q647G9
E	115	GLY	-	expression tag	UNP Q647G9
E	116	SER	-	expression tag	UNP Q647G9
E	117	HIS	-	expression tag	UNP Q647G9
E	118	HIS	-	expression tag	UNP Q647G9
E	119	HIS	-	expression tag	UNP Q647G9
E	120	HIS	-	expression tag	UNP Q647G9
E	121	HIS	-	expression tag	UNP Q647G9
E	122	HIS	-	expression tag	UNP Q647G9
G	1	MET	-	initiating methionine	UNP Q647G9
G	59	GLY	ARG	conflict	UNP Q647G9
G	91	SER	ASN	conflict	UNP Q647G9
G	114	SER	-	expression tag	UNP Q647G9
G	115	GLY	-	expression tag	UNP Q647G9
G	116	SER	-	expression tag	UNP Q647G9
G	117	HIS	-	expression tag	UNP Q647G9
G	118	HIS	-	expression tag	UNP Q647G9
G	119	HIS	-	expression tag	UNP Q647G9
G	120	HIS	-	expression tag	UNP Q647G9
G	121	HIS	-	expression tag	UNP Q647G9
G	122	HIS	-	expression tag	UNP Q647G9
F	1	MET	-	initiating methionine	UNP Q647G9
F	59	GLY	ARG	conflict	UNP Q647G9
F	91	SER	ASN	conflict	UNP Q647G9
F	114	SER	-	expression tag	UNP Q647G9
F	115	GLY	-	expression tag	UNP Q647G9
F	116	SER	-	expression tag	UNP Q647G9
F	117	HIS	-	expression tag	UNP Q647G9
F	118	HIS	-	expression tag	UNP Q647G9
F	119	HIS	-	expression tag	UNP Q647G9
F	120	HIS	-	expression tag	UNP Q647G9
F	121	HIS	-	expression tag	UNP Q647G9
F	122	HIS	-	expression tag	UNP Q647G9

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.

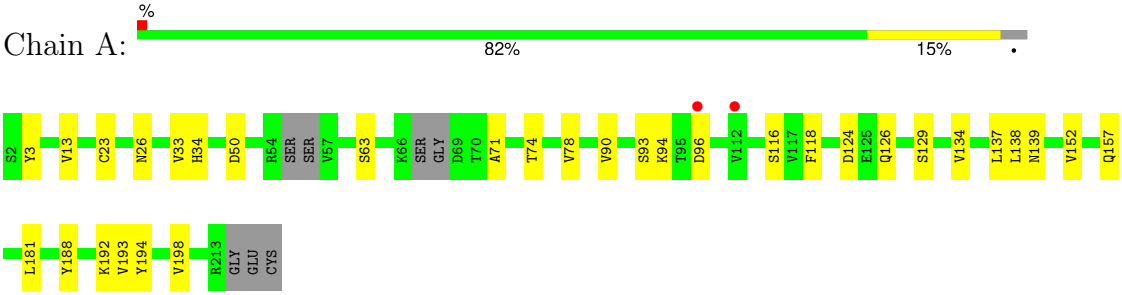
• Molecule 1: 16A8 Light Chain

Chain L:



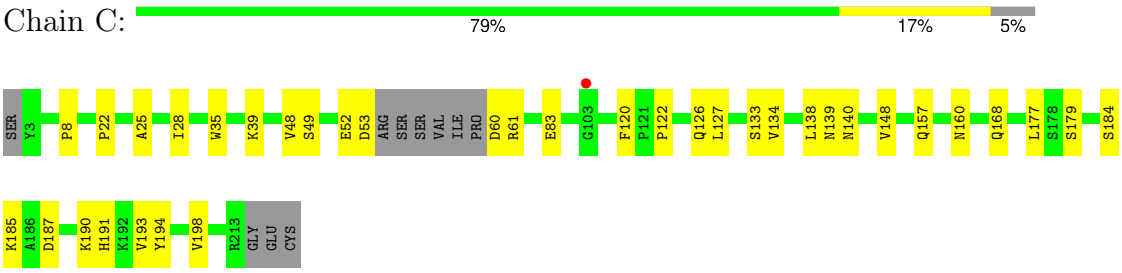
• Molecule 1: 16A8 Light Chain

Chain A:



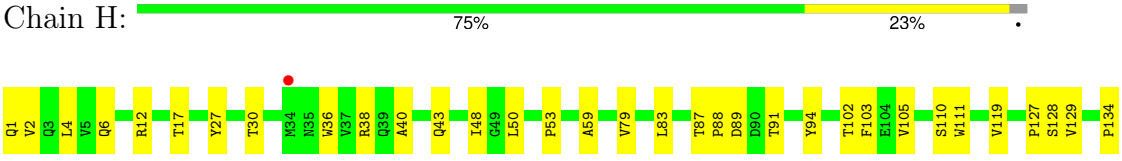
• Molecule 1: 16A8 Light Chain

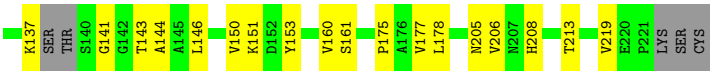
Chain C:



• Molecule 2: 16A8 Heavy Chain

Chain H:



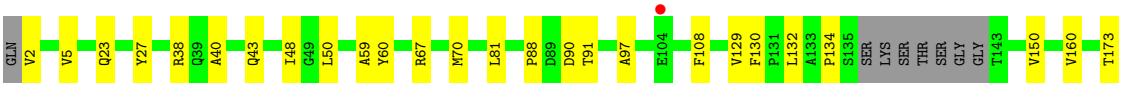


• Molecule 2: 16A8 Heavy Chain

Chain B:

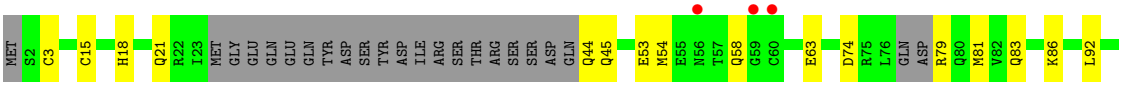
• Molecule 2: 16A8 Heavy Chain

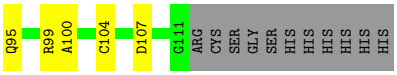
Chain D:



• Molecule 3: Conglutin

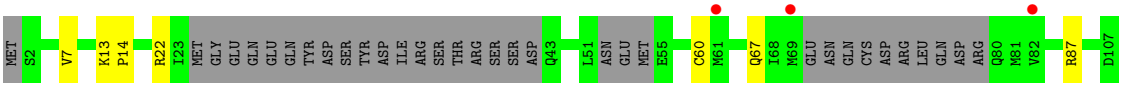
Chain E:





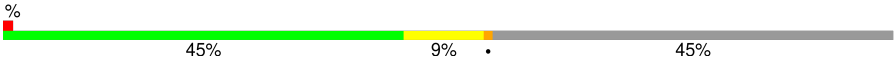
• Molecule 3: Conglutin

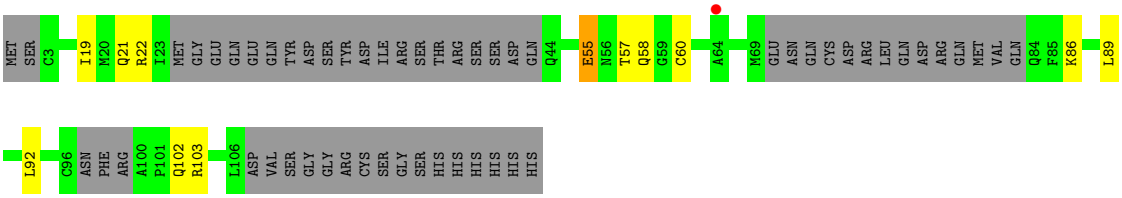
Chain G:



• Molecule 3: Conglutin

Chain F:




MET SER C3 I19 M20 Q21 R22 I23 MET GLY GLU GLN GLU GLN TYR ASP SER TYR ASP ILE ARG SER THR ARG SER SER ASP GLN Q44 E55 N56 T57 Q58 G59 C60 A64 M69 GLU ASN GLN CYS ASP ARG LEU GLN ASP ARG GLN MET VAL GLN Q84 F85 K86 L89

L92 C96 ASN PHE ARG A100 P101 Q102 R103 L106 ASP VAL SER GLY GLY ARG CYS SER GLY SER HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	105.55Å 155.31Å 286.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.78 – 3.20 52.78 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.6 (52.78-3.20) 92.6 (52.78-3.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.247 , 0.300 0.246 , 0.298	Depositor DCC
R_{free} test set	1859 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	104.8	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 108.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11439	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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

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	0.24	0/1629	0.48	0/2215
1	C	0.25	0/1600	0.48	0/2176
1	L	0.24	0/1605	0.47	0/2184
2	B	0.25	0/1656	0.49	0/2263
2	D	0.25	0/1616	0.49	0/2210
2	H	0.25	0/1687	0.49	0/2304
3	E	0.23	0/717	0.50	0/953
3	F	0.23	0/547	0.52	0/725
3	G	0.27	0/609	0.51	0/808
All	All	0.25	0/11666	0.49	0/15838

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1596	0	1550	18	0
1	C	1567	0	1514	19	0
1	L	1571	0	1529	25	0
2	B	1616	0	1564	24	0
2	D	1576	0	1520	22	0
2	H	1646	0	1595	33	0
3	E	714	0	682	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	546	0	526	8	0
3	G	607	0	584	2	0
All	All	11439	0	11064	152	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 7.

All (152) 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:143:THR:HG22	2:H:144:ALA:H	1.32	0.94
2:H:40:ALA:HB3	2:H:43:GLN:HB2	1.63	0.80
2:B:40:ALA:HB3	2:B:43:GLN:HB2	1.66	0.76
3:E:79:ARG:NH1	3:E:81:MET:SD	2.64	0.70
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.75	0.68
2:B:160:VAL:HG22	2:B:206:VAL:HG23	1.76	0.68
2:H:150:VAL:HG11	2:H:206:VAL:HG21	1.76	0.66
1:C:39:LYS:NZ	1:C:83:GLU:O	2.29	0.65
2:H:137:LYS:HD3	2:H:141:GLY:HA3	1.79	0.65
2:B:150:VAL:HG11	2:B:206:VAL:HG21	1.79	0.65
2:D:40:ALA:HB3	2:D:43:GLN:HB2	1.81	0.63
1:L:35:TRP:HB2	1:L:48:VAL:HG12	1.81	0.63
2:B:19:LYS:HG3	2:B:82:GLU:HG3	1.81	0.62
2:H:160:VAL:HG22	2:H:206:VAL:HG23	1.82	0.62
2:H:143:THR:HG22	2:H:144:ALA:N	2.11	0.61
1:C:191:HIS:ND1	1:C:193:VAL:HG12	2.16	0.60
2:H:87:THR:OG1	2:H:89:ASP:OD1	2.20	0.60
2:D:200:GLN:HG3	2:D:201:THR:H	1.68	0.58
2:D:38:ARG:HB3	2:D:48:ILE:HD11	1.85	0.58
2:B:38:ARG:HB3	2:B:48:ILE:HD11	1.84	0.58
1:L:28:ILE:HD11	1:L:90:VAL:HG11	1.86	0.57
1:L:162:GLN:NE2	2:H:178:LEU:O	2.32	0.57
3:G:7:VAL:HG11	3:G:67:GLN:HG3	1.87	0.57
1:C:148:VAL:HG22	1:C:198:VAL:HG12	1.87	0.56
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.39	0.56
1:L:25:ALA:HB3	1:L:28:ILE:HD13	1.87	0.56
2:B:61:ALA:HB3	2:B:64:PHE:HD2	1.70	0.56
2:D:129:VAL:HG22	2:D:150:VAL:HG12	1.88	0.56
2:D:150:VAL:HG11	2:D:206:VAL:HG21	1.88	0.55
2:B:129:VAL:HG22	2:B:150:VAL:HG12	1.88	0.55
2:D:160:VAL:HG22	2:D:206:VAL:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:N	1:A:124:ASP:OD1	2.40	0.55
1:A:138:LEU:HD21	1:A:198:VAL:HG21	1.88	0.54
1:L:116:SER:HB3	1:L:139:ASN:HB2	1.89	0.53
1:C:184:SER:OG	1:C:185:LYS:N	2.41	0.53
2:B:101:GLY:O	3:F:102:GLN:NE2	2.40	0.53
3:E:58:GLN:HG2	3:E:99:ARG:HB3	1.91	0.51
2:D:2:VAL:HG22	2:D:27:TYR:HB3	1.92	0.51
1:L:164:SER:HB2	2:H:175:PRO:HG2	1.92	0.51
2:B:5:VAL:O	2:B:23:GLN:N	2.44	0.51
2:H:134:PRO:HB3	2:H:146:LEU:HB3	1.93	0.50
1:C:126:GLN:NE2	1:C:133:SER:OG	2.34	0.50
1:L:92:ASP:OD2	1:L:95:THR:OG1	2.30	0.50
2:B:24:THR:HG1	2:B:27:TYR:HE1	1.59	0.50
2:D:176:ALA:HA	2:D:186:LEU:HB3	1.92	0.50
1:L:201:GLN:N	1:L:201:GLN:OE1	2.45	0.50
2:H:50:LEU:N	2:H:59:ALA:O	2.45	0.49
1:L:8:PRO:HG2	1:L:22:PRO:HD2	1.94	0.49
2:H:50:LEU:HB3	2:H:59:ALA:HB3	1.93	0.49
1:C:187:ASP:HB3	1:C:194:TYR:OH	2.13	0.49
1:C:157:GLN:HB3	1:C:160:ASN:HD21	1.79	0.48
2:D:70:MET:HE2	2:D:81:LEU:HD12	1.95	0.48
2:H:12:ARG:NH1	2:H:17:THR:O	2.47	0.48
1:A:63:SER:OG	1:A:74:THR:OG1	2.27	0.48
3:E:53:GLU:HA	3:E:54:MET:HA	1.59	0.47
1:C:35:TRP:HB2	1:C:48:VAL:HG22	1.96	0.47
3:G:13:LYS:HG3	3:G:14:PRO:HD3	1.97	0.47
1:L:7:GLN:NE2	1:L:86:TYR:O	2.43	0.46
1:A:23:CYS:N	1:A:71:ALA:O	2.49	0.46
2:D:60:TYR:HE1	2:D:70:MET:HG3	1.80	0.46
1:L:108:VAL:O	1:L:168:GLN:NE2	2.38	0.46
2:D:134:PRO:HG3	2:D:197:LEU:HD11	1.97	0.46
1:A:34:HIS:CD2	1:A:50:ASP:H	2.33	0.46
1:C:8:PRO:HG2	1:C:22:PRO:HD2	1.98	0.46
3:E:15:CYS:HA	3:E:18:HIS:HD2	1.81	0.46
2:H:102:THR:H	2:H:105:VAL:HG13	1.81	0.45
2:D:173:THR:HG23	2:D:188:SER:HB2	1.98	0.45
1:A:13:VAL:HG11	1:A:78:VAL:HG21	1.96	0.45
3:E:74:ASP:N	3:E:74:ASP:OD1	2.50	0.45
2:H:146:LEU:HD13	2:H:219:VAL:HG21	1.98	0.45
1:L:151:LYS:HG3	1:L:195:ALA:HB3	1.99	0.45
2:H:30:THR:HA	2:H:53:PRO:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:PRO:HG2	2:B:196:SER:HB3	1.99	0.45
3:E:92:LEU:HD12	3:E:95:GLN:HE21	1.82	0.44
2:H:4:LEU:HD22	2:H:110:SER:O	2.17	0.44
2:B:91:THR:HG22	2:B:119:VAL:H	1.82	0.44
1:L:135:VAL:HG13	1:L:180:THR:HG22	2.00	0.44
1:L:19:ALA:O	1:L:74:THR:HA	2.18	0.44
2:H:2:VAL:HG22	2:H:27:TYR:HB3	2.00	0.44
1:A:126:GLN:O	1:A:129:SER:OG	2.32	0.44
2:B:67:ARG:NH2	2:B:85:GLY:O	2.46	0.44
1:C:25:ALA:HB3	1:C:28:ILE:HB	1.98	0.44
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.99	0.44
2:B:167:LEU:HD21	2:B:190:VAL:HG21	1.98	0.44
2:H:1:GLN:OE1	2:H:1:GLN:N	2.49	0.44
1:A:118:PHE:HD2	1:A:137:LEU:HD22	1.82	0.44
3:F:19:ILE:HD11	3:F:92:LEU:HD22	2.00	0.44
3:F:86:LYS:HA	3:F:89:LEU:HB3	1.99	0.44
1:C:190:LYS:O	1:C:191:HIS:HB2	2.18	0.43
2:D:88:PRO:O	2:D:91:THR:HG22	2.18	0.43
3:E:18:HIS:HA	3:E:21:GLN:HG3	2.00	0.43
2:H:36:TRP:HE1	2:H:79:VAL:HG12	1.84	0.43
1:L:61:ARG:HD3	1:L:61:ARG:H	1.83	0.43
2:H:103:PHE:CE1	3:E:100:ALA:HB1	2.54	0.43
2:B:54:HIS:NE2	3:F:58:GLN:HG2	2.34	0.43
1:C:126:GLN:HG3	2:D:130:PHE:CE2	2.54	0.43
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.99	0.43
1:A:188:TYR:HA	1:A:194:TYR:OH	2.18	0.43
1:A:94:LYS:O	1:A:94:LYS:HG2	2.19	0.43
3:E:86:LYS:HD3	3:E:107:ASP:OD2	2.18	0.43
2:H:208:HIS:HB3	2:H:213:THR:HB	2.00	0.43
1:A:192:LYS:HA	1:A:192:LYS:HD3	1.73	0.43
2:B:199:THR:OG1	2:B:200:GLN:N	2.51	0.42
2:B:204:CYS:SG	2:B:217:LYS:HB3	2.58	0.42
2:D:5:VAL:O	2:D:23:GLN:N	2.41	0.42
3:E:86:LYS:NZ	3:E:107:ASP:OD1	2.36	0.42
1:A:152:VAL:HB	1:A:157:GLN:HE22	1.84	0.42
3:F:21:GLN:HE22	3:F:22:ARG:HG3	1.85	0.42
1:L:150:TRP:CG	1:L:181:LEU:HD13	2.54	0.42
1:A:33:VAL:HA	1:A:90:VAL:HG12	2.02	0.42
1:L:33:VAL:HA	1:L:90:VAL:HG12	2.00	0.42
1:A:34:HIS:ND1	2:B:107:TYR:HB3	2.35	0.42
2:H:6:GLN:NE2	2:H:94:TYR:O	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:91:THR:HB	2:H:119:VAL:HG12	2.02	0.42
1:A:116:SER:HB3	1:A:139:ASN:HB3	2.01	0.42
1:C:127:LEU:HD22	1:C:185:LYS:HE3	2.02	0.42
3:F:21:GLN:NE2	3:F:22:ARG:HG3	2.34	0.42
1:C:60:ASP:OD1	1:C:61:ARG:N	2.50	0.42
2:D:208:HIS:ND1	2:D:210:PRO:O	2.53	0.42
1:A:96:ASP:OD1	3:F:103:ARG:NH1	2.53	0.42
2:B:147:GLY:HA2	2:B:162:TRP:CZ2	2.55	0.42
1:L:36:TYR:CE2	1:L:89:GLN:HG2	2.55	0.41
3:E:44:GLN:HB3	3:E:45:GLN:H	1.59	0.41
2:H:88:PRO:O	2:H:91:THR:HG22	2.20	0.41
2:H:83:LEU:HD23	2:H:83:LEU:HA	1.91	0.41
2:B:23:GLN:HG2	2:B:78:THR:HG22	2.02	0.41
2:D:204:CYS:HB2	2:D:217:LYS:H	1.86	0.41
1:L:185:LYS:HE2	1:L:185:LYS:HB3	1.80	0.41
1:A:134:VAL:O	1:A:181:LEU:N	2.42	0.41
1:C:49:SER:OG	1:C:52:GLU:HB3	2.21	0.41
1:L:105:LYS:HA	1:L:105:LYS:HD2	1.90	0.41
2:H:151:LYS:HZ2	2:H:151:LYS:HG2	1.65	0.41
3:E:3:CYS:HB3	3:E:63:GLU:HG3	2.03	0.41
2:H:129:VAL:HG22	2:H:150:VAL:HG12	2.03	0.41
1:A:93:SER:O	1:A:94:LYS:HB3	2.21	0.41
2:D:50:LEU:N	2:D:59:ALA:O	2.53	0.41
3:F:55:GLU:HG2	3:F:57:THR:O	2.21	0.41
1:L:109:LEU:HD22	2:B:180:SER:HA	2.03	0.41
1:L:153:ASP:HA	1:L:193:VAL:HB	2.03	0.41
1:C:138:LEU:HD13	1:C:177:LEU:HD22	2.03	0.41
1:L:162:GLN:HE21	2:H:177:VAL:HG22	1.86	0.40
2:D:97:ALA:HB1	2:D:108:PHE:HB3	2.03	0.40
3:E:83:GLN:HA	3:E:86:LYS:HE2	2.03	0.40
1:L:44:PRO:HG2	2:H:111:TRP:CD2	2.57	0.40
2:B:30:THR:HA	2:B:53:PRO:HB2	2.03	0.40
1:L:123:SER:HB2	1:L:125:GLU:OE1	2.21	0.40
1:C:122:PRO:HG3	1:C:134:VAL:HG22	2.03	0.40
1:C:139:ASN:OD1	1:C:140:ASN:ND2	2.54	0.40
2:D:192:VAL:HG22	2:D:193:PRO:HD2	2.03	0.40
2:H:161:SER:O	2:H:205:ASN:HB2	2.21	0.40
2:B:51:ILE:HD12	2:B:70:MET:HB3	2.04	0.40
1:C:120:PHE:CD1	2:D:132:LEU:HB3	2.56	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	202/215 (94%)	194 (96%)	6 (3%)	2 (1%)	13 47
1	C	201/215 (94%)	196 (98%)	5 (2%)	0	100 100
1	L	202/215 (94%)	196 (97%)	6 (3%)	0	100 100
2	B	210/224 (94%)	202 (96%)	8 (4%)	0	100 100
2	D	205/224 (92%)	197 (96%)	8 (4%)	0	100 100
2	H	215/224 (96%)	205 (95%)	10 (5%)	0	100 100
3	E	82/122 (67%)	76 (93%)	6 (7%)	0	100 100
3	F	59/122 (48%)	55 (93%)	4 (7%)	0	100 100
3	G	66/122 (54%)	65 (98%)	1 (2%)	0	100 100
All	All	1442/1683 (86%)	1386 (96%)	54 (4%)	2 (0%)	48 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	193	VAL

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	A	182/187 (97%)	181 (100%)	1 (0%)	86 93
1	C	178/187 (95%)	175 (98%)	3 (2%)	56 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	179/187 (96%)	177 (99%)	2 (1%)	70 86
2	B	184/192 (96%)	180 (98%)	4 (2%)	47 73
2	D	179/192 (93%)	179 (100%)	0	100 100
2	H	187/192 (97%)	186 (100%)	1 (0%)	86 93
3	E	83/115 (72%)	82 (99%)	1 (1%)	67 85
3	F	64/115 (56%)	62 (97%)	2 (3%)	35 66
3	G	71/115 (62%)	68 (96%)	3 (4%)	25 58
All	All	1307/1482 (88%)	1290 (99%)	17 (1%)	65 83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	154	ASN
1	L	213	ARG
2	H	128	SER
1	A	3	TYR
2	B	89	ASP
2	B	106	TYR
2	B	135	SER
2	B	151	LYS
1	C	53	ASP
1	C	168	GLN
1	C	179	SER
3	E	104	CYS
3	G	22	ARG
3	G	60	CYS
3	G	87	ARG
3	F	55	GLU
3	F	60	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	52	ASN
2	D	113	GLN

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 oligosaccharides 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, 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	A	208/215 (96%)	0.01	2 (0%)	79	66	82, 126, 193, 286	0
1	C	205/215 (95%)	-0.13	1 (0%)	87	78	95, 131, 195, 233	0
1	L	206/215 (95%)	-0.12	3 (1%)	71	56	63, 111, 175, 234	0
2	B	214/224 (95%)	-0.13	0	100	100	73, 114, 166, 205	0
2	D	209/224 (93%)	-0.05	1 (0%)	87	78	94, 135, 195, 238	0
2	H	219/224 (97%)	-0.23	1 (0%)	87	78	61, 98, 170, 257	0
3	E	88/122 (72%)	0.31	3 (3%)	48	34	101, 178, 214, 258	0
3	F	67/122 (54%)	0.36	1 (1%)	71	56	146, 202, 270, 306	0
3	G	74/122 (60%)	0.43	3 (4%)	42	28	131, 194, 238, 268	0
All	All	1490/1683 (88%)	-0.04	15 (1%)	79	66	61, 127, 209, 306	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	64	ALA	3.6
3	G	61	MET	3.5
3	G	82	VAL	3.1
2	D	104	GLU	3.0
1	L	103	GLY	3.0
1	C	103	GLY	2.9
1	A	96	ASP	2.9
1	L	139	ASN	2.7
3	G	69	MET	2.4
3	E	56	ASN	2.4
1	L	20	SER	2.2
2	H	34	MET	2.2
1	A	112	VAL	2.1
3	E	59	GLY	2.1
3	E	60	CYS	2.1

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.