Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 05:18 AM EDT

PDB ID	:	7SBZ
Title	:	JAR5 Fab bound to fHbp v1.1 crystallized in space group I422
Authors	:	Chesterman, C.; Malito, E.; Bottomley, M.J.
Deposited on	:	2021-09-26
Resolution	:	2.90 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:

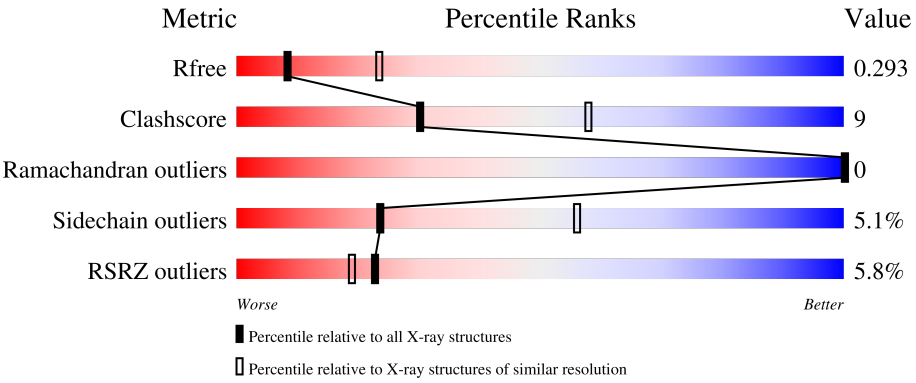
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	253	2% 69% 16% 13%
1	H	253	3% 67% 20% 13%
2	B	216	13% 75% 22%
2	L	216	10% 72% 22%
3	C	257	2% 69% 22% 7%

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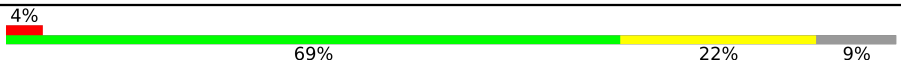
Mol	Chain	Length	Quality of chain
3	D	257	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10211 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 JAR5 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1675	1067	274	325	9			
1	H	221	Total	C	N	O	S	0	0	0
			1687	1073	276	330	8			

- Molecule 2 is a protein called JAR5 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1654	1037	278	331	8			
2	L	209	Total	C	N	O	S	0	0	0
			1617	1013	274	322	8			

- Molecule 3 is a protein called Factor H-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	239	Total	C	N	O	S	0	0	0
			1792	1111	322	358	1			
3	D	234	Total	C	N	O	S	0	0	0
			1761	1094	317	349	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	7	MET	-	initiating methionine	UNP E6MV22
C	256	LEU	-	expression tag	UNP E6MV22
C	257	GLU	-	expression tag	UNP E6MV22
C	258	HIS	-	expression tag	UNP E6MV22
C	259	HIS	-	expression tag	UNP E6MV22
C	260	HIS	-	expression tag	UNP E6MV22
C	261	HIS	-	expression tag	UNP E6MV22
C	262	HIS	-	expression tag	UNP E6MV22

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Chain	Residue	Modelled	Actual	Comment	Reference
C	263	HIS	-	expression tag	UNP E6MV22
D	7	MET	-	initiating methionine	UNP E6MV22
D	256	LEU	-	expression tag	UNP E6MV22
D	257	GLU	-	expression tag	UNP E6MV22
D	258	HIS	-	expression tag	UNP E6MV22
D	259	HIS	-	expression tag	UNP E6MV22
D	260	HIS	-	expression tag	UNP E6MV22
D	261	HIS	-	expression tag	UNP E6MV22
D	262	HIS	-	expression tag	UNP E6MV22
D	263	HIS	-	expression tag	UNP E6MV22

- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

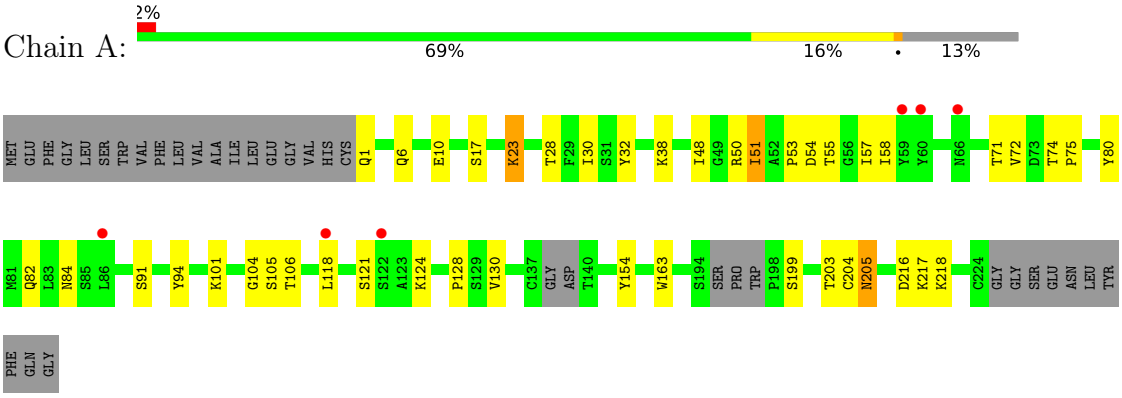
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cd 1 1	0	0
4	B	3	Total Cd 3 3	0	0
4	H	2	Total Cd 2 2	0	0
4	L	5	Total Cd 5 5	0	0
4	C	6	Total Cd 6 6	0	0
4	D	8	Total Cd 8 8	0	0

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.

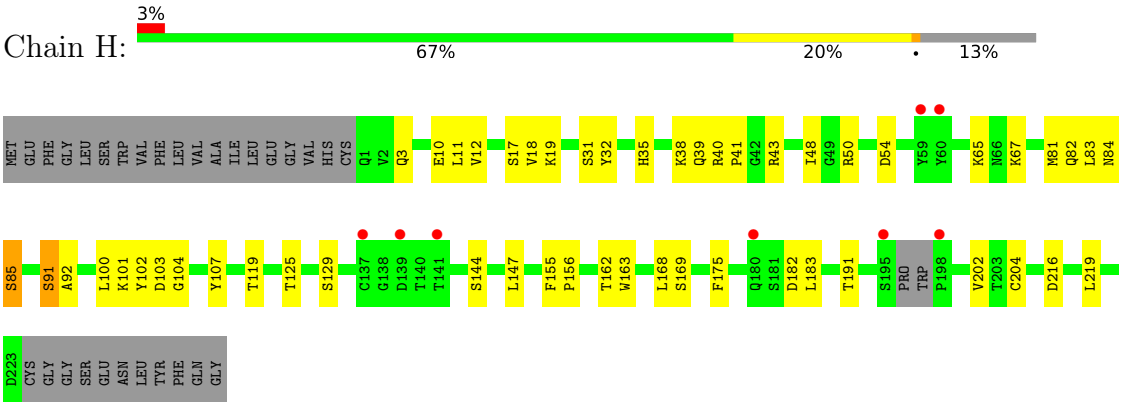
• Molecule 1: JAR5 Heavy Chain

Chain A:



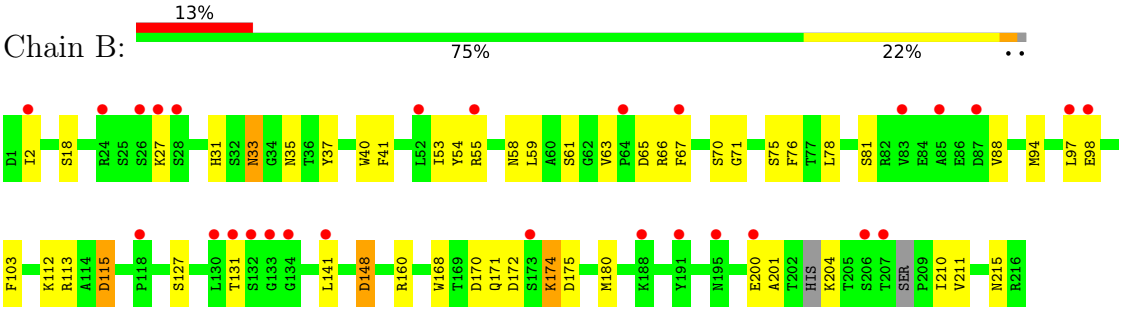
• Molecule 1: JAR5 Heavy Chain

Chain H:

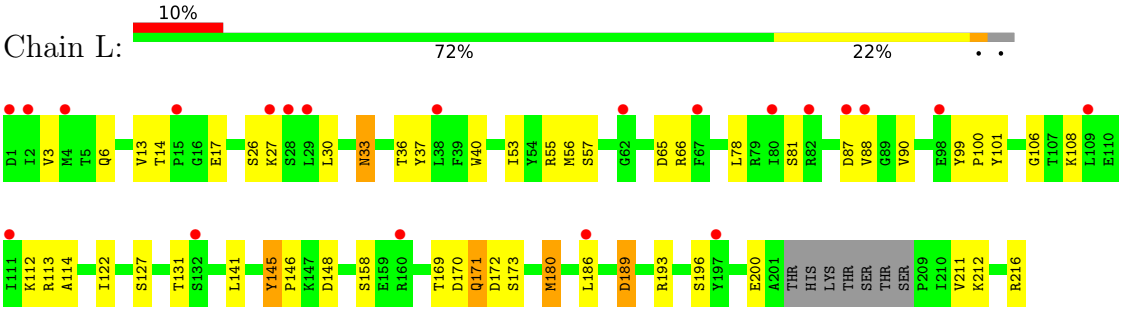


• Molecule 2: JAR5 Light Chain

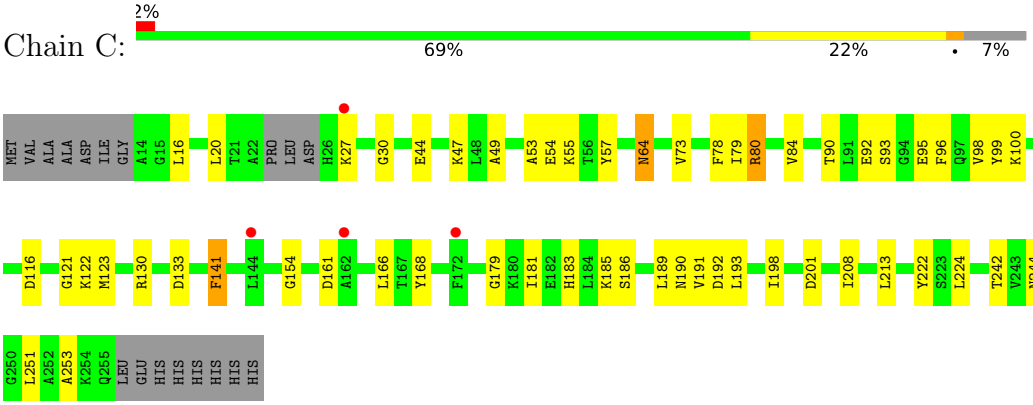
Chain B:



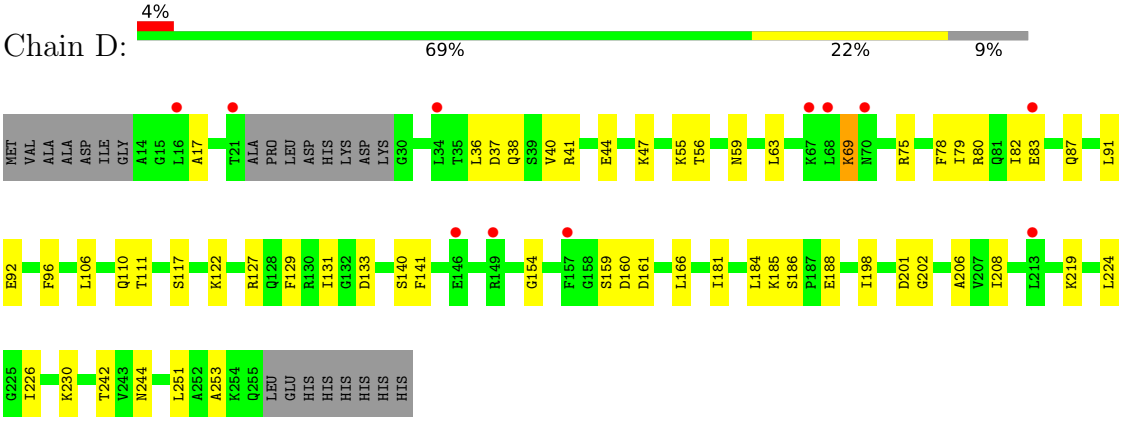
• Molecule 2: JAR5 Light Chain



• Molecule 3: Factor H-binding protein



• Molecule 3: Factor H-binding protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	167.66Å 167.66Å 313.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 2.90 49.27 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.27-2.90) 91.0 (49.27-2.90)	Depositor EDS
R_{merge}	0.58	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.86 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158)	Depositor
R, R_{free}	0.248 , 0.296 0.248 , 0.293	Depositor DCC
R_{free} test set	3818 reflections (7.70%)	wwPDB-VP
Wilson B-factor (Å^2)	71.4	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.0	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	0.90	EDS
Total number of atoms	10211	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6234e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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

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	0.26	0/1720	0.50	0/2348
1	H	0.26	0/1733	0.51	0/2367
2	B	0.26	0/1691	0.51	0/2293
2	L	0.28	0/1655	0.54	0/2246
3	C	0.27	0/1814	0.51	0/2433
3	D	0.26	0/1783	0.53	0/2390
All	All	0.27	0/10396	0.52	0/14077

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	1675	0	1644	26	0
1	H	1687	0	1652	32	0
2	B	1654	0	1593	35	0
2	L	1617	0	1546	35	0
3	C	1792	0	1769	36	0
3	D	1761	0	1752	36	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	0	0
4	C	6	0	0	0	0
4	D	8	0	0	0	0
4	H	2	0	0	0	0
4	L	5	0	0	0	0
All	All	10211	0	9956	187	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 (187) 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:40:TRP:HB2	2:B:53:ILE:HB	1.59	0.85
3:D:41:ARG:HB2	3:D:44:GLU:OE2	1.80	0.82
3:C:189:LEU:HD12	3:C:249:ILE:HD11	1.65	0.77
3:D:201:ASP:OD2	3:D:202:GLY:N	2.18	0.76
1:H:103:ASP:OD2	1:H:104:GLY:N	2.20	0.74
2:L:30:LEU:HD13	2:L:36:THR:HG22	1.70	0.74
3:D:83:GLU:OE2	3:D:83:GLU:N	2.17	0.74
1:A:105:SER:HA	3:D:87:GLN:HE22	1.51	0.74
1:A:51:ILE:HG12	1:A:58:ILE:HG12	1.70	0.74
2:L:14:THR:HG22	2:L:17:GLU:HB2	1.70	0.73
2:L:66:ARG:NH2	2:L:87:ASP:OD2	2.23	0.71
2:L:3:VAL:HG22	2:L:26:SER:HB3	1.72	0.70
2:B:148:ASP:HB3	2:B:204:LYS:HE3	1.74	0.70
3:C:78:PHE:HB3	3:C:96:PHE:HB2	1.75	0.68
1:H:40:ARG:HG2	1:H:41:PRO:HD2	1.76	0.68
3:C:47:LYS:HB2	3:C:79:ILE:HG23	1.75	0.67
2:B:59:LEU:HD12	2:B:63:VAL:HB	1.78	0.66
1:A:30:ILE:H	1:A:30:ILE:HD12	1.60	0.65
3:D:47:LYS:HB2	3:D:79:ILE:HG12	1.79	0.63
2:B:141:LEU:HD22	2:B:180:MET:HE2	1.79	0.63
3:D:166:LEU:HD22	3:D:251:LEU:HB3	1.81	0.63
2:L:40:TRP:HB2	2:L:53:ILE:HB	1.81	0.62
1:A:104:GLY:HA2	2:B:55:ARG:HH22	1.65	0.61
2:B:31:HIS:ND1	2:B:33:ASN:OD1	2.30	0.61
3:C:166:LEU:HD22	3:C:251:LEU:HB3	1.83	0.60
1:H:162:THR:HA	1:H:168:LEU:HD13	1.84	0.59
2:L:65:ASP:N	2:L:65:ASP:OD1	2.35	0.59
2:L:37:TYR:HE1	3:C:122:LYS:HG2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:79:ILE:HG13	3:C:90:THR:HG23	1.85	0.59
3:C:192:ASP:HB2	3:C:213:LEU:O	2.04	0.58
3:C:30:GLY:HA3	3:C:100:LYS:HE2	1.85	0.58
3:D:36:LEU:HD11	3:D:63:LEU:HB2	1.87	0.57
2:B:71:GLY:HA3	2:B:76:PHE:HA	1.87	0.57
1:A:53:PRO:HB3	1:A:72:VAL:HG21	1.88	0.56
2:L:112:LYS:HA	2:L:145:TYR:OH	2.05	0.56
1:H:17:SER:HA	1:H:83:LEU:O	2.05	0.56
2:L:200:GLU:HG3	2:L:211:VAL:HG22	1.88	0.56
2:L:189:ASP:OD2	2:L:189:ASP:N	2.38	0.56
1:A:55:THR:OG1	1:A:57:ILE:HG13	2.06	0.55
1:H:12:VAL:HG11	1:H:18:VAL:HB	1.88	0.55
1:A:38:LYS:HB2	1:A:48:ILE:HD11	1.89	0.54
2:B:113:ARG:HG2	2:B:113:ARG:HH11	1.71	0.54
2:B:33:ASN:HD22	2:B:35:ASN:H	1.54	0.54
3:C:141:PHE:CE1	3:C:198:ILE:HG22	2.43	0.54
1:H:10:GLU:OE2	1:H:10:GLU:HA	2.09	0.53
2:B:2:ILE:HD11	2:B:27:LYS:HD2	1.91	0.53
1:H:100:LEU:HD11	3:C:84:VAL:HG11	1.89	0.53
2:L:90:VAL:HG22	2:L:108:LYS:HG3	1.90	0.53
1:H:147:LEU:HB3	1:H:219:LEU:HD13	1.90	0.53
2:B:127:SER:O	2:B:131:THR:HG23	2.08	0.53
1:H:163:TRP:HZ3	1:H:219:LEU:HD11	1.73	0.53
2:L:216:ARG:HG2	2:L:216:ARG:HH11	1.73	0.53
2:B:40:TRP:CG	2:B:78:LEU:HD13	2.44	0.53
2:L:88:VAL:HG21	2:L:171:GLN:HB3	1.90	0.53
1:H:54:ASP:OD1	1:H:101:LYS:NZ	2.41	0.52
3:D:161:ASP:OD2	3:D:185:LYS:N	2.40	0.52
3:D:17:ALA:HB3	3:D:55:LYS:HE2	1.92	0.52
3:D:92:GLU:OE1	3:D:111:THR:OG1	2.22	0.52
3:D:78:PHE:HB3	3:D:96:PHE:HB2	1.92	0.52
1:A:101:LYS:HD2	3:D:117:SER:HB2	1.92	0.52
1:H:48:ILE:HG21	1:H:81:MET:HE2	1.91	0.52
3:D:40:VAL:O	3:D:59:ASN:ND2	2.35	0.51
3:D:106:LEU:HD12	3:D:131:ILE:HD11	1.92	0.51
1:A:10:GLU:OE2	1:A:10:GLU:HA	2.10	0.51
1:H:38:LYS:HB2	1:H:48:ILE:HD11	1.91	0.51
2:L:55:ARG:O	2:L:56:MET:HG3	2.11	0.51
1:H:31:SER:O	1:H:101:LYS:HG2	2.09	0.51
3:C:191:VAL:HG22	3:C:192:ASP:H	1.76	0.51
2:B:37:TYR:CE1	3:D:122:LYS:HD3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:208:ILE:HG13	3:D:224:LEU:HB2	1.93	0.50
3:C:44:GLU:OE1	3:C:80:ARG:NH1	2.44	0.50
1:H:17:SER:HB3	1:H:82:GLN:HE21	1.76	0.50
3:D:206:ALA:HB1	3:D:226:ILE:HD12	1.93	0.50
3:C:92:GLU:OE2	3:C:130:ARG:NH2	2.43	0.50
3:D:141:PHE:HE2	3:D:198:ILE:HG22	1.75	0.50
2:B:201:ALA:HB3	2:B:210:ILE:HG13	1.94	0.50
3:C:186:SER:HB2	3:C:189:LEU:HD23	1.92	0.50
1:H:144:SER:HB2	1:H:191:THR:HG22	1.92	0.50
3:C:49:ALA:HB2	3:C:54:GLU:HG3	1.92	0.49
3:C:181:ILE:HD12	3:C:191:VAL:HG12	1.95	0.49
1:H:216:ASP:OD1	1:H:216:ASP:N	2.39	0.49
2:L:13:VAL:O	2:L:112:LYS:N	2.40	0.49
3:C:98:VAL:HG22	3:C:107:THR:HG22	1.93	0.49
2:B:88:VAL:HG21	2:B:171:GLN:HB2	1.94	0.49
3:C:154:GLY:HA3	3:C:253:ALA:HA	1.93	0.49
2:L:6:GLN:OE1	2:L:106:GLY:N	2.46	0.49
3:D:127:ARG:NH2	3:D:160:ASP:OD1	2.46	0.49
2:L:113:ARG:HG2	2:L:114:ALA:N	2.28	0.48
2:L:146:PRO:HG2	2:L:148:ASP:OD2	2.12	0.48
3:C:242:THR:HG23	3:C:244:ASN:H	1.78	0.48
2:L:148:ASP:OD2	2:L:148:ASP:N	2.43	0.48
1:H:3:GLN:HE21	1:H:3:GLN:HA	1.79	0.48
1:A:128:PRO:HB3	1:A:154:TYR:HB3	1.95	0.48
3:D:82:ILE:HB	3:D:91:LEU:HD11	1.96	0.48
1:H:101:LYS:HE3	1:H:102:TYR:CZ	2.49	0.47
1:A:105:SER:HA	3:D:87:GLN:NE2	2.26	0.47
3:D:188:GLU:OE1	3:D:242:THR:OG1	2.32	0.47
1:A:71:THR:OG1	1:A:80:TYR:HB2	2.15	0.47
2:B:54:TYR:CE2	2:B:58:ASN:HB2	2.49	0.47
3:C:109:PHE:HB2	3:C:130:ARG:HG3	1.95	0.47
3:D:17:ALA:HB1	3:D:55:LYS:HB2	1.96	0.47
1:H:103:ASP:OD1	2:L:37:TYR:OH	2.29	0.47
2:B:65:ASP:N	2:B:65:ASP:OD1	2.47	0.47
1:H:32:TYR:HE2	1:H:107:TYR:HB3	1.79	0.47
2:L:66:ARG:HB3	2:L:81:SER:O	2.15	0.47
3:D:47:LYS:HG2	3:D:56:THR:HG23	1.97	0.46
1:H:182:ASP:O	1:H:183:LEU:HD23	2.15	0.46
2:B:70:SER:OG	2:B:71:GLY:N	2.47	0.46
3:D:242:THR:HG23	3:D:244:ASN:H	1.80	0.46
3:C:55:LYS:HG2	3:C:57:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLN:NE2	1:A:94:TYR:O	2.48	0.46
2:L:112:LYS:HA	2:L:145:TYR:HH	1.81	0.46
2:L:127:SER:O	2:L:131:THR:HG23	2.16	0.46
1:H:202:VAL:HG13	1:H:219:LEU:HB2	1.98	0.45
2:L:141:LEU:HD23	2:L:180:MET:HE3	1.98	0.45
1:H:175:PHE:CD1	2:L:169:THR:HG23	2.51	0.45
2:B:66:ARG:HB2	2:B:81:SER:HB2	1.98	0.45
1:H:50:ARG:NH2	2:L:99:TYR:OH	2.49	0.45
3:D:154:GLY:HA3	3:D:253:ALA:HA	1.99	0.45
2:L:145:TYR:CD2	2:L:146:PRO:HA	2.52	0.45
3:D:129:PHE:HB2	3:D:159:SER:OG	2.17	0.45
3:D:44:GLU:OE1	3:D:80:ARG:NE	2.50	0.45
1:H:85:SER:O	1:H:85:SER:OG	2.27	0.45
3:C:193:LEU:HD12	3:C:222:TYR:CG	2.52	0.44
1:A:17:SER:HB3	1:A:82:GLN:NE2	2.32	0.44
3:C:193:LEU:HD12	3:C:222:TYR:CD2	2.52	0.44
1:A:23:LYS:HE2	1:A:23:LYS:HB2	1.82	0.44
1:A:106:THR:HG22	2:B:54:TYR:CZ	2.53	0.44
1:A:130:VAL:HB	1:A:217:LYS:HD3	1.99	0.44
1:H:54:ASP:C	1:H:54:ASP:OD2	2.56	0.44
1:A:124:LYS:HE3	1:A:124:LYS:HB2	1.60	0.44
3:C:64:ASN:HD22	3:C:64:ASN:C	2.22	0.43
3:C:95:GLU:HB3	3:C:110:GLN:HB3	1.99	0.43
1:H:91:SER:OG	1:H:119:THR:HA	2.17	0.43
1:A:104:GLY:HA2	2:B:55:ARG:NH2	2.33	0.43
1:A:163:TRP:CZ3	1:A:204:CYS:HB3	2.54	0.43
1:H:35:HIS:CE1	2:L:101:TYR:HE1	2.36	0.43
3:C:208:ILE:HG23	3:C:224:LEU:HB2	2.01	0.43
1:A:91:SER:HA	1:A:118:LEU:O	2.18	0.43
2:L:113:ARG:HB3	2:L:145:TYR:CD1	2.54	0.43
2:L:189:ASP:O	2:L:193:ARG:HG2	2.19	0.43
2:B:53:ILE:HD11	2:B:59:LEU:HD22	2.00	0.43
3:C:73:VAL:HG22	3:C:99:TYR:HD1	1.83	0.43
3:D:219:LYS:HD2	3:D:219:LYS:HA	1.67	0.43
1:H:67:LYS:O	1:H:83:LEU:HA	2.18	0.42
3:D:141:PHE:CE2	3:D:198:ILE:HG22	2.54	0.42
1:A:1:GLN:HA	1:A:1:GLN:OE1	2.20	0.42
1:A:74:THR:N	1:A:75:PRO:HD2	2.34	0.42
2:B:41:PHE:CZ	2:B:94:MET:HE2	2.54	0.42
2:B:168:TRP:CD1	2:B:180:MET:HG3	2.54	0.42
3:D:161:ASP:HB2	3:D:185:LYS:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:99:TYR:N	2:L:100:PRO:HD2	2.34	0.42
3:C:181:ILE:HG13	3:C:193:LEU:HD21	2.02	0.42
3:D:181:ILE:HD11	3:D:251:LEU:HD21	2.01	0.42
3:C:116:ASP:O	3:C:121:GLY:HA2	2.20	0.42
1:A:28:THR:O	1:A:32:TYR:HD1	2.01	0.42
2:L:27:LYS:HB2	2:L:27:LYS:HE2	1.93	0.42
3:C:49:ALA:HA	3:C:53:ALA:O	2.20	0.42
2:L:122:ILE:HB	2:L:212:LYS:HE3	2.02	0.42
2:B:172:ASP:OD1	2:B:174:LYS:HD3	2.20	0.42
3:C:183:HIS:H	3:C:190:ASN:HD21	1.68	0.42
2:B:18:SER:OG	2:B:81:SER:O	2.20	0.41
2:B:59:LEU:HD21	2:B:67:PHE:O	2.20	0.41
2:L:180:MET:HE3	2:L:180:MET:HB3	1.65	0.41
3:D:185:LYS:HG3	3:D:186:SER:N	2.34	0.41
2:B:2:ILE:HD13	2:B:2:ILE:HA	1.87	0.41
1:H:39:GLN:O	1:H:92:ALA:HB1	2.19	0.41
2:B:115:ASP:N	2:B:115:ASP:OD1	2.54	0.41
2:B:160:ARG:HA	2:B:160:ARG:HD3	1.87	0.41
3:C:247:ARG:HA	3:C:247:ARG:HD2	1.80	0.41
2:B:53:ILE:HD13	2:B:53:ILE:HA	1.80	0.41
2:B:97:LEU:HG	2:B:98:GLU:HG3	2.02	0.41
3:D:37:ASP:O	3:D:59:ASN:ND2	2.50	0.41
3:C:16:LEU:HD22	3:C:20:LEU:HG	2.03	0.41
3:C:161:ASP:CG	3:C:185:LYS:HG2	2.41	0.41
2:B:33:ASN:ND2	2:B:35:ASN:H	2.19	0.41
2:B:94:MET:HB2	2:B:103:PHE:CD1	2.56	0.41
2:B:200:GLU:HB2	2:B:211:VAL:HG12	2.02	0.41
1:H:11:LEU:HB2	1:H:156:PRO:HG3	2.02	0.41
2:L:33:ASN:O	2:L:33:ASN:ND2	2.52	0.41
3:D:69:LYS:HB2	3:D:69:LYS:HE2	1.88	0.41
3:D:184:LEU:HD12	3:D:184:LEU:HA	1.86	0.41
1:A:205:ASN:HD22	1:A:216:ASP:CG	2.24	0.40
3:C:123:MET:HE2	3:C:123:MET:HB2	1.91	0.40
1:A:54:ASP:C	1:A:54:ASP:OD2	2.60	0.40
1:H:155:PHE:HA	1:H:156:PRO:HA	1.93	0.40
3:C:168:TYR:CD2	3:C:179:GLY:HA3	2.57	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	213/253 (84%)	210 (99%)	3 (1%)	0	100	100
1	H	217/253 (86%)	206 (95%)	11 (5%)	0	100	100
2	B	208/216 (96%)	199 (96%)	9 (4%)	0	100	100
2	L	205/216 (95%)	192 (94%)	13 (6%)	0	100	100
3	C	235/257 (91%)	230 (98%)	5 (2%)	0	100	100
3	D	230/257 (90%)	226 (98%)	4 (2%)	0	100	100
All	All	1308/1452 (90%)	1263 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	190/217 (88%)	181 (95%)	9 (5%)	26	59
1	H	191/217 (88%)	181 (95%)	10 (5%)	23	55
2	B	189/192 (98%)	179 (95%)	10 (5%)	22	54
2	L	183/192 (95%)	170 (93%)	13 (7%)	14	40
3	C	182/200 (91%)	174 (96%)	8 (4%)	28	61
3	D	180/200 (90%)	173 (96%)	7 (4%)	32	66
All	All	1115/1218 (92%)	1058 (95%)	57 (5%)	24	56

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

Mol	Chain	Res	Type
1	A	23	LYS
1	A	50	ARG
1	A	51	ILE
1	A	84	ASN
1	A	121	SER
1	A	199	SER
1	A	203	THR
1	A	205	ASN
1	A	218	LYS
2	B	33	ASN
2	B	61	SER
2	B	75	SER
2	B	112	LYS
2	B	115	ASP
2	B	148	ASP
2	B	170	ASP
2	B	174	LYS
2	B	175	ASP
2	B	215	ASN
1	H	19	LYS
1	H	43	ARG
1	H	65	LYS
1	H	84	ASN
1	H	85	SER
1	H	91	SER
1	H	125	THR
1	H	129	SER
1	H	169	SER
1	H	204	CYS
2	L	33	ASN
2	L	57	SER
2	L	78	LEU
2	L	145	TYR
2	L	158	SER
2	L	170	ASP
2	L	171	GLN
2	L	172	ASP
2	L	173	SER
2	L	180	MET
2	L	186	LEU
2	L	189	ASP
2	L	196	SER

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Mol	Chain	Res	Type
3	C	27	LYS
3	C	64	ASN
3	C	80	ARG
3	C	93	SER
3	C	133	ASP
3	C	141	PHE
3	C	201	ASP
3	C	247	ARG
3	D	38	GLN
3	D	69	LYS
3	D	75	ARG
3	D	110	GLN
3	D	133	ASP
3	D	140	SER
3	D	230	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	35	ASN
2	B	161	GLN
2	B	166	ASN
2	B	171	GLN
1	H	3	GLN
2	L	47	GLN
3	C	64	ASN
3	C	70	ASN
3	C	183	HIS
3	D	87	GLN
3	D	176	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 25 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	219/253 (86%)	0.25	6 (2%) 54 50	53, 77, 109, 130	0
1	H	221/253 (87%)	0.26	8 (3%) 42 37	44, 77, 118, 138	0
2	B	214/216 (99%)	0.74	28 (13%) 3 2	60, 88, 111, 142	0
2	L	209/216 (96%)	0.62	21 (10%) 7 5	54, 86, 111, 121	0
3	C	239/257 (92%)	0.27	4 (1%) 70 69	47, 73, 105, 125	0
3	D	234/257 (91%)	0.40	11 (4%) 31 28	53, 80, 116, 130	0
All	All	1336/1452 (92%)	0.42	78 (5%) 23 19	44, 80, 112, 142	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	130	LEU	4.3
2	B	67	PHE	3.8
2	B	132	SER	3.8
3	D	34	LEU	3.8
2	B	85	ALA	3.8
2	L	28	SER	3.7
2	L	27	LYS	3.6
2	L	2	ILE	3.6
1	H	195	SER	3.5
2	B	83	VAL	3.5
1	H	137	CYS	3.4
2	L	38	LEU	3.3
3	D	83	GLU	3.2
2	B	64	PRO	3.2
2	B	27	LYS	3.2
2	B	173	SER	3.2
2	B	2	ILE	3.2
2	L	111	ILE	3.1
2	L	67	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	195	ASN	3.0
2	B	87	ASP	3.0
2	L	4	MET	3.0
2	B	98	GLU	3.0
2	L	132	SER	3.0
2	L	197	TYR	3.0
2	L	87	ASP	2.9
2	L	109	LEU	2.9
1	H	60	TYR	2.9
2	L	29	LEU	2.9
3	D	67	LYS	2.9
2	L	98	GLU	2.8
1	A	60	TYR	2.8
2	B	134	GLY	2.7
3	C	172	PHE	2.7
3	D	68	LEU	2.6
2	B	118	PRO	2.6
2	L	80	ILE	2.6
2	B	200	GLU	2.6
3	C	27	LYS	2.6
2	B	26	SER	2.6
1	H	141	THR	2.6
2	L	88	VAL	2.6
2	L	82	ARG	2.5
3	C	144	LEU	2.5
1	A	66	ASN	2.5
2	B	52	LEU	2.5
2	B	206	SER	2.5
3	C	162	ALA	2.5
2	B	28	SER	2.4
2	B	97	LEU	2.4
2	B	55	ARG	2.4
3	D	213	LEU	2.4
1	H	59	TYR	2.4
1	A	118	LEU	2.3
2	B	188	LYS	2.3
1	A	59	TYR	2.3
1	A	86	LEU	2.3
2	B	207	THR	2.3
2	B	24	ARG	2.3
2	B	133	GLY	2.2
1	H	139	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	186	LEU	2.2
3	D	157	PHE	2.2
1	H	198	PRO	2.2
1	H	180	GLN	2.2
2	L	1	ASP	2.2
3	D	16	LEU	2.2
2	L	62	GLY	2.2
3	D	149	ARG	2.2
3	D	70	ASN	2.1
2	B	131	THR	2.1
3	D	146	GLU	2.1
2	L	15	PRO	2.1
1	A	122	SER	2.1
3	D	21	THR	2.1
2	L	160	ARG	2.1
2	B	141	LEU	2.0
2	B	191	TYR	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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CD	D	305	1/1	0.56	0.08	186,186,186,186	0
4	CD	L	305	1/1	0.61	0.33	334,334,334,334	0
4	CD	C	302	1/1	0.65	0.10	193,193,193,193	0
4	CD	C	305	1/1	0.70	0.22	153,153,153,153	1
4	CD	L	303	1/1	0.70	0.11	178,178,178,178	0
4	CD	D	307	1/1	0.71	0.13	166,166,166,166	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CD	A	301	1/1	0.72	0.14	130,130,130,130	1
4	CD	H	301	1/1	0.79	0.18	151,151,151,151	1
4	CD	C	304	1/1	0.80	0.25	134,134,134,134	1
4	CD	B	303	1/1	0.81	0.05	156,156,156,156	0
4	CD	C	303	1/1	0.85	0.11	184,184,184,184	0
4	CD	D	306	1/1	0.87	0.07	182,182,182,182	0
4	CD	B	301	1/1	0.87	0.12	174,174,174,174	0
4	CD	D	304	1/1	0.88	0.07	186,186,186,186	0
4	CD	D	303	1/1	0.88	0.17	158,158,158,158	1
4	CD	D	301	1/1	0.89	0.12	141,141,141,141	0
4	CD	B	302	1/1	0.89	0.07	167,167,167,167	0
4	CD	C	306	1/1	0.90	0.11	148,148,148,148	0
4	CD	L	302	1/1	0.92	0.05	180,180,180,180	0
4	CD	L	301	1/1	0.92	0.16	134,134,134,134	1
4	CD	H	302	1/1	0.93	0.16	100,100,100,100	1
4	CD	L	304	1/1	0.94	0.21	139,139,139,139	0
4	CD	C	301	1/1	0.96	0.10	112,112,112,112	1
4	CD	D	308	1/1	0.97	0.16	161,161,161,161	1
4	CD	D	302	1/1	0.98	0.17	143,143,143,143	0

6.5 Other polymers (i)

There are no such residues in this entry.