Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2021 – 04:21 PM EDT

PDB ID	:	6XH5
Title	:	Hierarchical design of multi-scale protein complexes by combinatorial assembly of oligomeric helical bundle and repeat protein building blocks
Authors	:	Bera, A.K.; Hsia, Y.; Kang, A.S.; Baker, D.
Deposited on	:	2020-06-18
Resolution	:	3.32 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

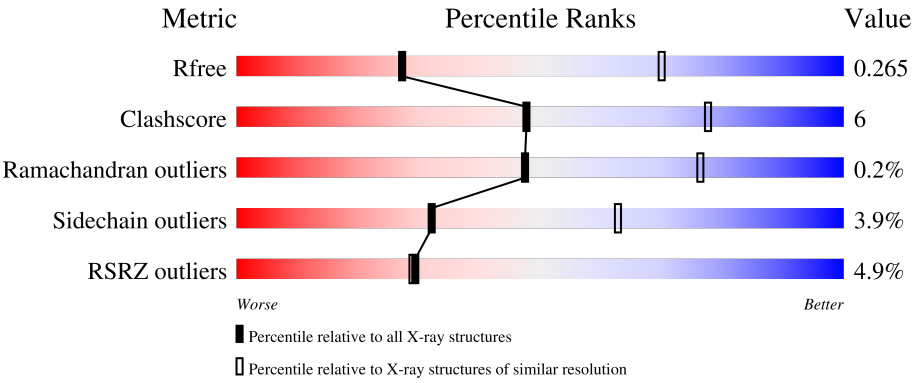
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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 3.32 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	359	81% 15%
1	B	359	12% 74% 21%
1	C	359	3% 82% 14%
1	D	359	3% 85% 10%
1	E	359	8% 79% 16%

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Mol	Chain	Length	Quality of chain
1	F	359	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15880 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 helical fusion design.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2653	1672	464	510	7			
1	B	348	Total	C	N	O	S	0	0	0
			2600	1639	451	503	7			
1	C	348	Total	C	N	O	S	0	0	0
			2645	1669	465	504	7			
1	D	348	Total	C	N	O	S	0	0	0
			2658	1675	465	511	7			
1	E	348	Total	C	N	O	S	0	0	0
			2624	1654	456	507	7			
1	F	348	Total	C	N	O	S	0	0	0
			2654	1672	464	511	7			

- Molecule 2 is water.

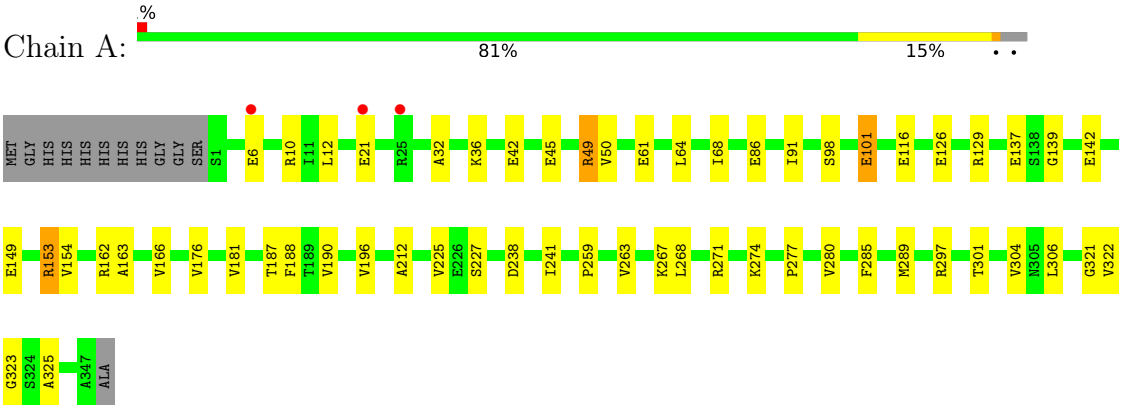
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	4	Total	O	0	0
			4	4		
2	C	7	Total	O	0	0
			7	7		
2	D	11	Total	O	0	0
			11	11		
2	E	6	Total	O	0	0
			6	6		
2	F	8	Total	O	0	0
			8	8		

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.

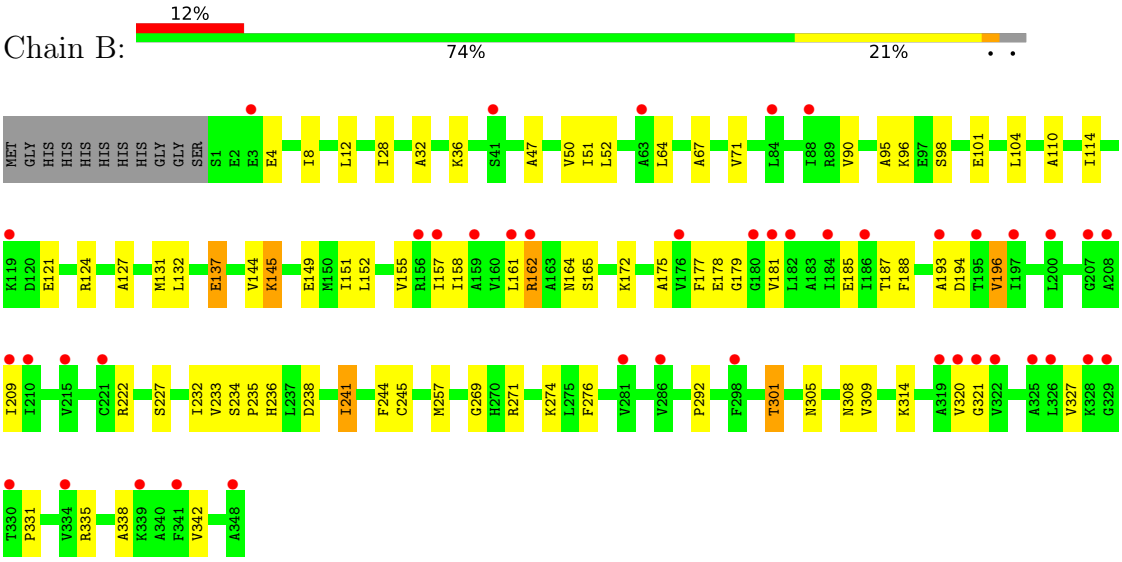
• Molecule 1: helical fusion design

Chain A:



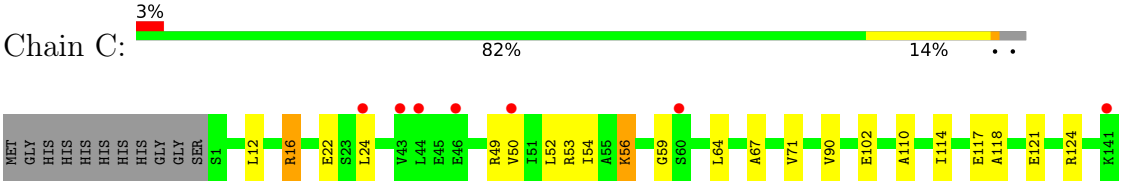
• Molecule 1: helical fusion design

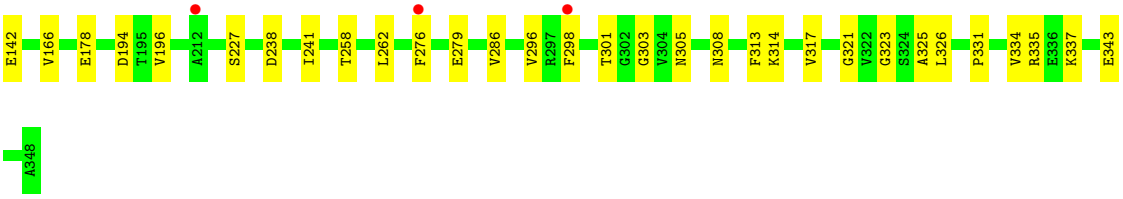
Chain B:



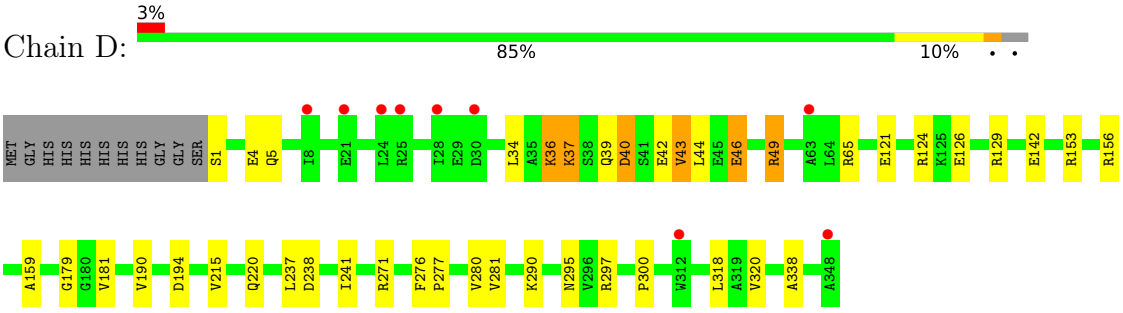
• Molecule 1: helical fusion design

Chain C:

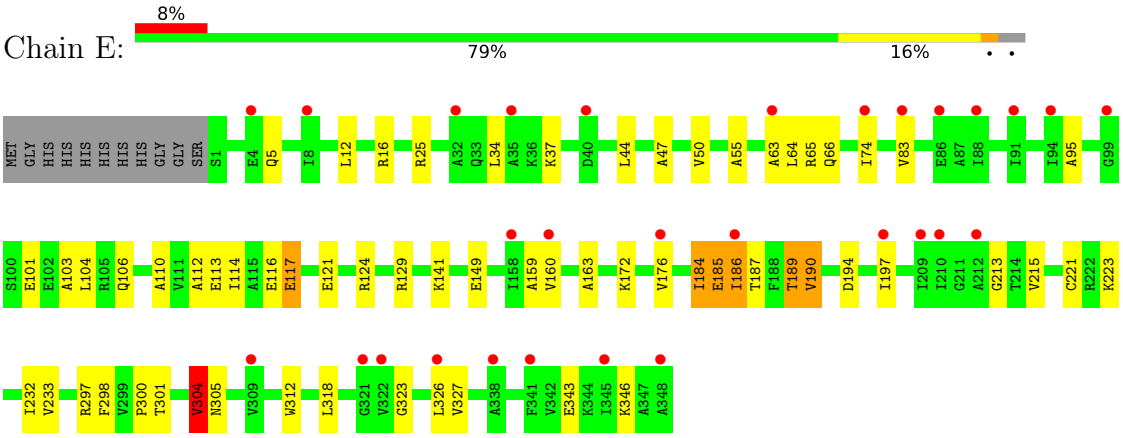




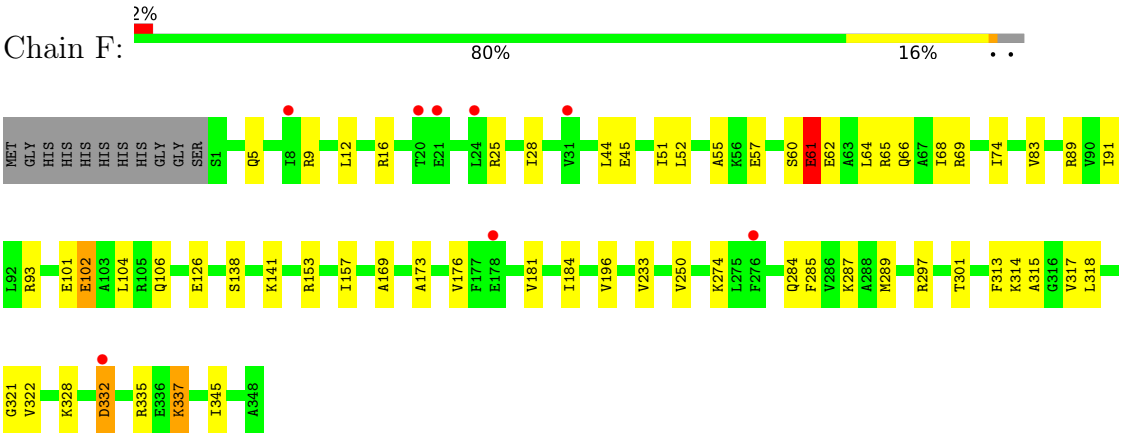
• Molecule 1: helical fusion design



• Molecule 1: helical fusion design



• Molecule 1: helical fusion design



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	166.77Å 166.77Å 223.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.12 – 3.32 78.12 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.9 (78.12-3.32) 99.9 (78.12-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.18rc2_3793	Depositor
R, R_{free}	0.219 , 0.265 0.219 , 0.265	Depositor DCC
R_{free} test set	2334 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	116.5	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 69.8	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	0.93	EDS
Total number of atoms	15880	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.82% 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	0/2679	0.37	0/3603
1	B	0.24	0/2626	0.39	0/3542
1	C	0.25	0/2671	0.40	0/3594
1	D	0.25	0/2684	0.39	0/3610
1	E	0.27	0/2650	0.43	0/3571
1	F	0.25	0/2680	0.38	0/3606
All	All	0.25	0/15990	0.39	0/21526

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	2653	0	2766	31	0
1	B	2600	0	2653	45	0
1	C	2645	0	2756	32	0
1	D	2658	0	2771	20	0
1	E	2624	0	2701	37	0
1	F	2654	0	2760	37	0
2	A	10	0	0	0	0
2	B	4	0	0	0	0
2	C	7	0	0	0	0
2	D	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	6	0	0	1	0
2	F	8	0	0	0	0
All	All	15880	0	16407	195	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 6.

All (195) 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)
1:E:160:VAL:HA	1:E:185:GLU:HB3	1.48	0.95
1:D:36:LYS:HG2	1:D:37:LYS:HG3	1.60	0.83
1:C:142:GLU:HG3	1:F:62:GLU:HG2	1.67	0.77
1:C:22:GLU:HB3	1:F:141:LYS:HE2	1.65	0.76
1:D:1:SER:HB3	1:D:40:ASP:OD2	1.88	0.74
1:D:5:GLN:NE2	1:D:46:GLU:OE2	2.21	0.74
1:C:102:GLU:OE2	1:F:65:ARG:NH1	2.22	0.72
1:E:163:ALA:H	1:E:190:VAL:HG23	1.56	0.69
1:C:118:ALA:HB1	1:C:124:ARG:HH11	1.57	0.68
1:D:36:LYS:HD2	1:D:37:LYS:HE2	1.75	0.68
1:B:101:GLU:HG2	1:B:104:LEU:HD12	1.75	0.67
1:F:28:ILE:HG23	1:F:51:ILE:HD11	1.77	0.67
1:F:60:SER:O	1:F:61:GLU:HB3	1.95	0.66
1:E:172:LYS:HD3	1:E:327:VAL:HG13	1.79	0.65
1:B:181:VAL:HG12	1:B:342:VAL:HG23	1.79	0.64
1:A:301:THR:HG22	1:A:321:GLY:HA3	1.78	0.64
1:B:145:LYS:NZ	1:B:269:GLY:O	2.31	0.63
1:A:49:ARG:NH1	1:A:86:GLU:OE2	2.32	0.62
1:F:68:ILE:HG23	1:F:91:ILE:HD12	1.82	0.62
1:F:89:ARG:NH1	1:F:126:GLU:OE2	2.34	0.61
1:C:178:GLU:OE1	1:C:335:ARG:NH1	2.34	0.61
1:B:238:ASP:OD1	1:B:241:ILE:N	2.21	0.61
1:B:149:GLU:OE1	1:B:271:ARG:NH1	2.33	0.60
1:B:151:ILE:HG21	1:B:209:ILE:HD12	1.82	0.60
1:C:262:LEU:HD21	1:C:296:VAL:HG21	1.83	0.60
1:B:96:LYS:NZ	1:B:137:GLU:OE2	2.32	0.60
1:B:132:LEU:HD11	1:B:209:ILE:HG12	1.84	0.59
1:A:12:LEU:HD12	1:A:50:VAL:HG13	1.84	0.59
1:C:334:VAL:HA	1:C:337:LYS:HG2	1.86	0.58
1:E:101:GLU:H	1:E:104:LEU:HD12	1.70	0.57
1:E:160:VAL:HA	1:E:185:GLU:CB	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:HD11	1:B:90:VAL:HG22	1.86	0.57
1:C:50:VAL:O	1:C:54:ILE:HG13	2.05	0.57
1:D:194:ASP:N	1:D:194:ASP:OD1	2.38	0.56
1:E:95:ALA:HB1	1:E:104:LEU:HD23	1.86	0.56
1:B:95:ALA:HB1	1:B:104:LEU:HD23	1.85	0.56
1:F:313:PHE:HA	1:F:317:VAL:HG12	1.88	0.56
1:E:343:GLU:HA	1:E:346:LYS:HE3	1.88	0.56
1:E:194:ASP:OD2	1:E:223:LYS:NZ	2.29	0.56
1:B:12:LEU:HD11	1:B:50:VAL:HG22	1.87	0.56
1:D:4:GLU:HB3	1:D:34:LEU:HD11	1.86	0.56
1:D:300:PRO:HG2	1:D:320:VAL:HG23	1.88	0.55
1:E:34:LEU:HB3	1:E:37:LYS:HA	1.88	0.55
1:B:193:ALA:HA	1:B:196:VAL:HG23	1.88	0.55
1:B:101:GLU:HA	1:B:104:LEU:HB2	1.89	0.55
1:C:301:THR:HG22	1:C:321:GLY:HA3	1.88	0.55
1:F:328:LYS:HB2	1:F:337:LYS:NZ	2.23	0.54
1:B:305:ASN:H	1:B:308:ASN:HB2	1.72	0.54
1:C:194:ASP:O	1:C:227:SER:OG	2.25	0.54
1:B:162:ARG:HD3	1:B:187:THR:HG21	1.89	0.54
1:C:102:GLU:OE2	1:F:102:GLU:HG3	2.08	0.53
1:A:126:GLU:HG3	1:A:129:ARG:HH12	1.73	0.53
1:F:25:ARG:NH1	1:F:66:GLN:HB3	2.23	0.53
1:F:62:GLU:OE1	1:F:62:GLU:N	2.42	0.53
1:E:112:ALA:O	1:E:116:GLU:HG3	2.09	0.53
1:F:52:LEU:HD21	1:F:93:ARG:CZ	2.39	0.53
1:D:297:ARG:HE	1:D:318:LEU:HD13	1.74	0.53
1:E:44:LEU:HG	1:E:83:VAL:HG21	1.90	0.53
1:E:159:ALA:O	1:E:185:GLU:N	2.40	0.52
1:B:127:ALA:O	1:B:131:MET:HG3	2.10	0.52
1:B:233:VAL:O	1:B:234:SER:HB3	2.09	0.52
1:A:149:GLU:OE2	1:A:297:ARG:NH2	2.38	0.52
1:E:55:ALA:HB1	1:E:64:LEU:HD23	1.92	0.52
1:A:163:ALA:H	1:A:190:VAL:HG22	1.75	0.52
1:B:161:LEU:HG	1:B:327:VAL:HG11	1.91	0.52
1:B:233:VAL:HG13	1:B:274:LYS:HD2	1.92	0.52
1:A:68:ILE:HG23	1:A:91:ILE:HD12	1.93	0.51
1:D:280:VAL:HG12	1:F:284:GLN:HG3	1.92	0.51
1:A:42:GLU:HA	1:A:45:GLU:HG2	1.93	0.50
1:C:313:PHE:HA	1:C:317:VAL:HG22	1.94	0.50
1:B:158:ILE:HD11	1:B:185:GLU:HB2	1.93	0.50
1:E:213:GLY:HA2	1:E:233:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:HD12	1:C:90:VAL:HG13	1.93	0.50
1:B:274:LYS:HE2	1:B:276:PHE:HB2	1.94	0.50
1:E:215:VAL:HG11	1:E:232:ILE:HG23	1.94	0.50
1:B:151:ILE:HD13	1:B:209:ILE:HD11	1.93	0.50
1:F:301:THR:HG22	1:F:321:GLY:HA3	1.93	0.50
1:A:304:VAL:HB	1:A:322:VAL:HG12	1.93	0.49
1:C:323:GLY:O	1:C:325:ALA:N	2.42	0.49
1:C:59:GLY:HA3	1:C:64:LEU:H	1.78	0.49
1:A:263:VAL:HG12	1:A:267:LYS:HE3	1.95	0.49
1:B:331:PRO:O	1:B:335:ARG:HG3	2.13	0.48
1:C:305:ASN:H	1:C:308:ASN:HB2	1.77	0.48
1:B:12:LEU:HD21	1:B:50:VAL:HG13	1.94	0.48
1:B:121:GLU:HG2	1:B:124:ARG:NH2	2.28	0.48
1:E:215:VAL:HG21	1:E:221:CYS:HB2	1.94	0.48
1:F:45:GLU:HG3	1:F:83:VAL:HG22	1.96	0.48
1:C:118:ALA:HB1	1:C:124:ARG:NH1	2.28	0.48
1:A:225:VAL:C	1:A:227:SER:H	2.17	0.48
1:A:274:LYS:HE3	1:A:301:THR:OG1	2.13	0.48
1:F:328:LYS:HB2	1:F:337:LYS:HZ1	1.77	0.48
1:A:323:GLY:O	1:A:325:ALA:N	2.45	0.47
1:F:16:ARG:HG2	1:F:57:GLU:OE1	2.15	0.47
1:E:25:ARG:NH1	1:E:66:GLN:OE1	2.48	0.47
1:A:61:GLU:OE1	1:A:98:SER:OG	2.30	0.46
1:A:166:VAL:HG13	1:A:196:VAL:HG22	1.97	0.46
1:F:297:ARG:HE	1:F:318:LEU:HD13	1.79	0.46
1:E:44:LEU:HA	1:E:47:ALA:HB3	1.97	0.46
1:E:106:GLN:NE2	2:E:401:HOH:O	2.47	0.46
1:E:187:THR:HG22	1:E:189:THR:HG23	1.98	0.46
1:F:233:VAL:HG13	1:F:274:LYS:HD2	1.97	0.46
1:B:175:ALA:HA	1:B:335:ARG:HE	1.81	0.46
1:E:65:ARG:HG3	1:E:103:ALA:HB2	1.97	0.46
1:A:162:ARG:HE	1:A:187:THR:HG21	1.79	0.46
1:C:53:ARG:HG2	1:C:53:ARG:HH11	1.80	0.46
1:F:176:VAL:HG22	1:F:181:VAL:HB	1.97	0.46
1:A:116:GLU:HG3	1:A:153:ARG:CZ	2.45	0.46
1:B:157:ILE:HG23	1:B:181:VAL:HB	1.98	0.46
1:D:121:GLU:HG2	1:D:124:ARG:NH2	2.31	0.46
1:E:25:ARG:HD3	1:E:63:ALA:HB2	1.98	0.46
1:B:194:ASP:O	1:B:227:SER:OG	2.29	0.45
1:E:12:LEU:HD12	1:E:50:VAL:HG13	1.98	0.45
1:F:285:PHE:O	1:F:289:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:GLY:HA3	1:B:338:ALA:HB3	1.98	0.45
1:E:172:LYS:O	1:E:176:VAL:HG22	2.17	0.45
1:E:176:VAL:CG2	1:E:184:ILE:HD11	2.46	0.45
1:C:56:LYS:HB3	1:C:56:LYS:HE2	1.33	0.45
1:B:52:LEU:HD21	1:B:90:VAL:HG13	1.98	0.45
1:B:172:LYS:HD3	1:B:327:VAL:HG12	1.99	0.45
1:F:69:ARG:HG2	1:F:106:GLN:HE22	1.81	0.44
1:F:157:ILE:HD11	1:F:345:ILE:HD12	1.98	0.44
1:D:49:ARG:HE	1:D:49:ARG:HB2	1.55	0.44
1:E:149:GLU:OE2	1:E:297:ARG:NH2	2.36	0.44
1:A:188:PHE:HE1	1:A:212:ALA:HB1	1.82	0.44
1:A:306:LEU:H	1:A:306:LEU:HD12	1.83	0.44
1:E:110:ALA:O	1:E:114:ILE:HG12	2.17	0.44
1:E:186:ILE:HG13	1:E:197:ILE:HG22	1.99	0.44
1:A:6:GLU:O	1:A:10:ARG:HG2	2.18	0.43
1:C:110:ALA:O	1:C:114:ILE:HG12	2.17	0.43
1:C:286:VAL:HG23	1:C:298:PHE:HD2	1.83	0.43
1:F:153:ARG:O	1:F:153:ARG:NE	2.50	0.43
1:C:117:GLU:H	1:C:117:GLU:HG2	1.61	0.43
1:A:149:GLU:CD	1:A:271:ARG:HH12	2.22	0.43
1:E:113:GLU:O	1:E:117:GLU:HG2	2.18	0.43
1:F:169:ALA:HB3	1:F:196:VAL:HG21	2.00	0.43
1:D:215:VAL:HA	1:D:220:GLN:NE2	2.33	0.43
1:D:159:ALA:HB2	1:D:181:VAL:HG11	2.00	0.43
1:F:102:GLU:H	1:F:102:GLU:HG2	1.28	0.43
1:A:32:ALA:O	1:A:36:LYS:HG3	2.19	0.43
1:B:4:GLU:O	1:B:8:ILE:HG12	2.18	0.43
1:C:279:GLU:HB3	1:C:303:GLY:H	1.83	0.43
1:B:309:VAL:HG23	1:B:320:VAL:HG21	2.01	0.43
1:C:166:VAL:HG13	1:C:196:VAL:HG22	2.01	0.43
1:D:276:PHE:HA	1:D:277:PRO:HA	1.90	0.43
1:D:43:VAL:HG12	1:D:44:LEU:HD23	2.00	0.42
1:F:61:GLU:HA	1:F:64:LEU:HB2	2.01	0.42
1:C:12:LEU:HD21	1:C:16:ARG:NH2	2.34	0.42
1:D:271:ARG:NE	1:D:295:ASN:O	2.53	0.42
1:A:176:VAL:HG22	1:A:181:VAL:HB	2.00	0.42
1:B:32:ALA:O	1:B:36:LYS:HG3	2.20	0.42
1:B:222:ARG:HG2	1:B:244:PHE:CZ	2.55	0.42
1:E:141:LYS:HB2	1:E:141:LYS:HE2	1.80	0.42
1:F:287:LYS:HG3	1:F:315:ALA:HB1	2.02	0.42
1:B:301:THR:HB	1:B:321:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLU:O	1:A:139:GLY:N	2.49	0.42
1:C:326:LEU:HD12	1:C:337:LYS:HG3	2.02	0.42
1:E:121:GLU:O	1:E:124:ARG:N	2.53	0.42
1:E:34:LEU:HD13	1:E:74:ILE:HG12	2.01	0.41
1:F:44:LEU:HD22	1:F:74:ILE:HG23	2.01	0.41
1:B:28:ILE:HG12	1:B:51:ILE:HG23	2.01	0.41
1:A:277:PRO:HB2	1:A:280:VAL:HG23	2.02	0.41
1:D:238:ASP:HB3	1:D:241:ILE:HB	2.02	0.41
1:E:186:ILE:HD13	1:E:186:ILE:HA	1.79	0.41
1:E:186:ILE:HG22	1:E:187:THR:O	2.20	0.41
1:F:332:ASP:O	1:F:335:ARG:NH2	2.53	0.41
1:A:64:LEU:HD13	1:A:98:SER:HB2	2.01	0.41
1:B:47:ALA:O	1:B:51:ILE:HG13	2.19	0.41
1:F:5:GLN:O	1:F:9:ARG:HG2	2.20	0.41
1:A:101:GLU:OE2	1:A:142:GLU:HB2	2.20	0.41
1:A:116:GLU:OE2	1:A:154:VAL:HA	2.20	0.41
1:B:145:LYS:HE2	1:B:145:LYS:HB3	1.90	0.41
1:C:67:ALA:O	1:C:71:VAL:HG12	2.20	0.41
1:B:67:ALA:O	1:B:71:VAL:HG12	2.20	0.41
1:B:110:ALA:O	1:B:114:ILE:HG12	2.20	0.41
1:C:49:ARG:O	1:C:53:ARG:HB2	2.19	0.41
1:E:160:VAL:CA	1:E:185:GLU:HB3	2.35	0.41
1:B:152:LEU:HA	1:B:155:VAL:HG22	2.03	0.41
1:D:179:GLY:HA3	1:D:338:ALA:HB3	2.03	0.41
1:F:104:LEU:HD13	1:F:138:SER:HB2	2.02	0.41
1:A:238:ASP:HB3	1:A:241:ILE:HB	2.02	0.41
1:C:12:LEU:HD21	1:C:16:ARG:HH22	1.85	0.41
1:F:314:LYS:HD3	1:F:314:LYS:HA	1.91	0.41
1:F:61:GLU:HA	1:F:64:LEU:HD12	2.03	0.40
1:F:173:ALA:HB1	1:F:184:ILE:HD13	2.03	0.40
1:A:259:PRO:HD3	1:B:257:MET:HE3	2.03	0.40
1:A:285:PHE:O	1:A:289:MET:HG2	2.21	0.40
1:C:331:PRO:HA	1:C:334:VAL:HG22	2.03	0.40
1:D:126:GLU:HG3	1:D:129:ARG:HH21	1.86	0.40
1:E:300:PRO:HG3	1:E:312:TRP:CE3	2.55	0.40
1:B:64:LEU:HD13	1:B:98:SER:HB2	2.03	0.40
1:B:292:PRO:HG3	1:C:276:PHE:HZ	1.86	0.40
1:D:142:GLU:OE1	1:D:142:GLU:N	2.50	0.40
1:E:304:VAL:HB	1:E:305:ASN:H	1.62	0.40
1:F:55:ALA:HB1	1:F:64:LEU:HD23	2.02	0.40
1:C:238:ASP:HB3	1:C:241:ILE:HB	2.04	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	345/359 (96%)	330 (96%)	15 (4%)	0	100 100
1	B	346/359 (96%)	331 (96%)	14 (4%)	1 (0%)	41 71
1	C	346/359 (96%)	331 (96%)	15 (4%)	0	100 100
1	D	346/359 (96%)	335 (97%)	10 (3%)	1 (0%)	41 71
1	E	346/359 (96%)	325 (94%)	19 (6%)	2 (1%)	25 57
1	F	346/359 (96%)	329 (95%)	16 (5%)	1 (0%)	41 71
All	All	2075/2154 (96%)	1981 (96%)	89 (4%)	5 (0%)	47 76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	304	VAL
1	D	40	ASP
1	F	61	GLU
1	B	235	PRO
1	E	323	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	A	278/286 (97%)	273 (98%)	5 (2%)	59 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	264/286 (92%)	248 (94%)	16 (6%)	18 49
1	C	274/286 (96%)	267 (97%)	7 (3%)	46 72
1	D	278/286 (97%)	264 (95%)	14 (5%)	24 56
1	E	270/286 (94%)	256 (95%)	14 (5%)	23 55
1	F	277/286 (97%)	269 (97%)	8 (3%)	42 70
All	All	1641/1716 (96%)	1577 (96%)	64 (4%)	32 63

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	49	ARG
1	A	101	GLU
1	A	153	ARG
1	A	268	LEU
1	B	137	GLU
1	B	144	VAL
1	B	145	LYS
1	B	162	ARG
1	B	164	ASN
1	B	165	SER
1	B	177	PHE
1	B	178	GLU
1	B	188	PHE
1	B	196	VAL
1	B	232	ILE
1	B	236	HIS
1	B	241	ILE
1	B	245	CYS
1	B	301	THR
1	B	314	LYS
1	C	16	ARG
1	C	24	LEU
1	C	56	LYS
1	C	121	GLU
1	C	258	THR
1	C	314	LYS
1	C	343	GLU
1	D	36	LYS
1	D	37	LYS

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Mol	Chain	Res	Type
1	D	39	GLN
1	D	42	GLU
1	D	43	VAL
1	D	46	GLU
1	D	49	ARG
1	D	65	ARG
1	D	153	ARG
1	D	156	ARG
1	D	190	VAL
1	D	237	LEU
1	D	281	VAL
1	D	290	LYS
1	E	5	GLN
1	E	16	ARG
1	E	117	GLU
1	E	129	ARG
1	E	184	ILE
1	E	185	GLU
1	E	186	ILE
1	E	189	THR
1	E	190	VAL
1	E	298	PHE
1	E	301	THR
1	E	304	VAL
1	E	318	LEU
1	E	326	LEU
1	F	12	LEU
1	F	61	GLU
1	F	101	GLU
1	F	102	GLU
1	F	250	VAL
1	F	322	VAL
1	F	332	ASP
1	F	337	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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, 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	347/359 (96%)	0.28	3 (0%) 84 85	69, 96, 136, 155	14 (4%)
1	B	348/359 (96%)	0.71	43 (12%) 4 3	89, 146, 183, 213	140 (40%)
1	C	348/359 (96%)	0.31	10 (2%) 51 51	76, 107, 143, 161	32 (9%)
1	D	348/359 (96%)	0.29	9 (2%) 56 53	68, 91, 141, 160	19 (5%)
1	E	348/359 (96%)	0.57	29 (8%) 11 11	84, 132, 174, 206	64 (18%)
1	F	348/359 (96%)	0.36	8 (2%) 60 59	68, 116, 144, 184	45 (12%)
All	All	2087/2154 (96%)	0.42	102 (4%) 29 29	68, 116, 164, 213	314 (15%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	348	ALA	5.3
1	E	341	PHE	4.6
1	B	180	GLY	4.5
1	C	60	SER	4.4
1	E	212	ALA	4.3
1	B	119	LYS	4.2
1	B	197	ILE	4.2
1	B	200	LEU	4.1
1	E	186	ILE	4.0
1	B	329	GLY	4.0
1	E	197	ILE	3.9
1	B	221	CYS	3.9
1	B	181	VAL	3.8
1	B	319	ALA	3.7
1	B	330	THR	3.7
1	B	210	ILE	3.7
1	E	160	VAL	3.6
1	B	195	THR	3.6
1	E	99	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	83	VAL	3.5
1	C	24	LEU	3.5
1	B	208	ALA	3.5
1	B	326	LEU	3.4
1	B	157	ILE	3.3
1	B	322	VAL	3.3
1	B	321	GLY	3.3
1	F	276	PHE	3.1
1	E	86	GLU	3.1
1	B	348	ALA	3.1
1	E	326	LEU	3.1
1	E	210	ILE	3.0
1	B	320	VAL	3.0
1	C	44	LEU	3.0
1	E	88	ILE	3.0
1	D	8	ILE	2.9
1	A	6	GLU	2.9
1	D	348	ALA	2.8
1	D	30	ASP	2.8
1	B	161	LEU	2.8
1	F	21	GLU	2.8
1	E	94	ILE	2.7
1	B	182	LEU	2.7
1	B	328	LYS	2.7
1	F	24	LEU	2.7
1	B	156	ARG	2.7
1	D	312	TRP	2.7
1	B	207	GLY	2.7
1	E	32	ALA	2.7
1	E	309	VAL	2.6
1	B	325	ALA	2.6
1	E	158	ILE	2.6
1	C	50	VAL	2.6
1	B	88	ILE	2.6
1	C	141	LYS	2.6
1	B	341	PHE	2.5
1	A	25	ARG	2.5
1	B	334	VAL	2.5
1	C	276	PHE	2.5
1	D	21	GLU	2.5
1	B	41	SER	2.5
1	E	338	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	184	ILE	2.5
1	B	159	ALA	2.5
1	E	345	ILE	2.4
1	E	35	ALA	2.4
1	C	43	VAL	2.4
1	D	25	ARG	2.4
1	B	186	ILE	2.3
1	B	286	VAL	2.3
1	E	176	VAL	2.3
1	E	74	ILE	2.3
1	D	28	ILE	2.3
1	E	91	ILE	2.3
1	B	176	VAL	2.3
1	B	3	GLU	2.3
1	F	31	VAL	2.3
1	E	321	GLY	2.3
1	D	24	LEU	2.2
1	F	332	ASP	2.2
1	B	298	PHE	2.2
1	E	322	VAL	2.2
1	B	193	ALA	2.2
1	B	162	ARG	2.2
1	E	4	GLU	2.2
1	B	84	LEU	2.2
1	E	63	ALA	2.2
1	B	281	VAL	2.2
1	C	298	PHE	2.1
1	D	63	ALA	2.1
1	C	46	GLU	2.1
1	E	8	ILE	2.1
1	F	8	ILE	2.1
1	A	21	GLU	2.1
1	B	215	VAL	2.1
1	B	339	LYS	2.1
1	E	40	ASP	2.1
1	C	212	ALA	2.0
1	B	209	ILE	2.0
1	F	178	GLU	2.0
1	E	209	ILE	2.0
1	F	20	THR	2.0
1	B	63	ALA	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.