Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 09:48 PM JST

PDB ID	:	6AEE
Title	:	Crystal structure of the four Ig-like domains of LILRB1 complexed with HLA-G
Authors	:	Wang, Q.; Song, H.; Qi, J.; Gao, G.F.
Deposited on	:	2018-08-04
Resolution	:	3.30 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:

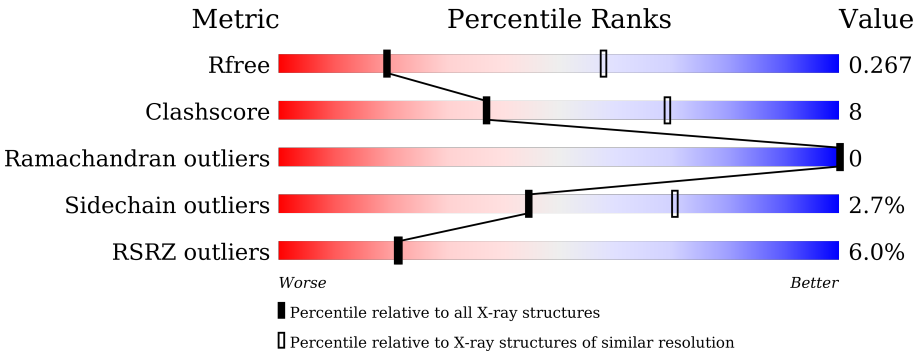
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	277	80% 16%
1	D	277	81% 18%
2	B	100	87% 13%
2	E	100	85% 15%
3	C	9	89% 11%
3	F	9	89% 11%

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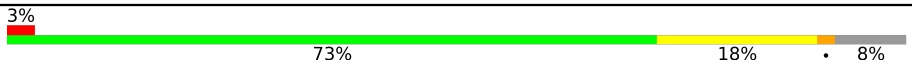
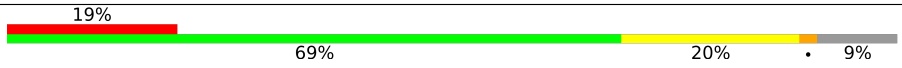
Mol	Chain	Length	Quality of chain
4	G	399	
4	H	399	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12038 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 HLA class I histocompatibility antigen, alpha chain G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2242	1397	404	429	12			
1	D	275	Total	C	N	O	S	0	0	0
			2242	1397	404	429	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P17693
A	42	SER	CYS	engineered mutation	UNP P17693
A	110	ILE	LEU	engineered mutation	UNP P17693
A	115	ARG	GLN	engineered mutation	UNP P17693
D	0	MET	-	initiating methionine	UNP P17693
D	42	SER	CYS	engineered mutation	UNP P17693
D	110	ILE	LEU	engineered mutation	UNP P17693
D	115	ARG	GLN	engineered mutation	UNP P17693

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1A	MET	-	initiating methionine	UNP P61769
E	1A	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called 9 Mer Peptide (RL9) From Histone H2A.x.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total 81	C 52	N 18	O 11	0	0	0
3	F	9	Total 81	C 52	N 18	O 11	0	0	0

- Molecule 4 is a protein called Leukocyte immunoglobulin-like receptor subfamily B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	369	Total 2887	C 1828	N 491	O 556	S 12	0	0	0
4	H	362	Total 2831	C 1796	N 481	O 542	S 12	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

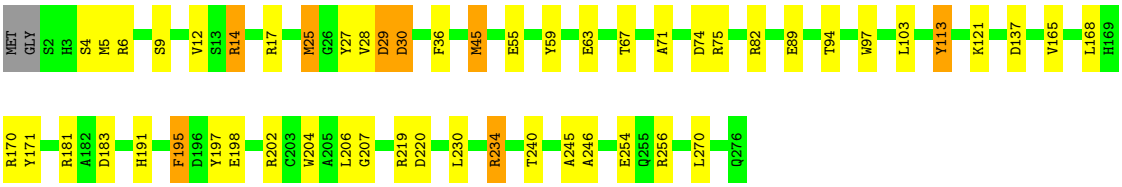
Chain	Residue	Modelled	Actual	Comment	Reference
G	395	HIS	-	expression tag	UNP A0A0G2JQ44
G	396	HIS	-	expression tag	UNP A0A0G2JQ44
G	397	HIS	-	expression tag	UNP A0A0G2JQ44
G	398	HIS	-	expression tag	UNP A0A0G2JQ44
G	399	HIS	-	expression tag	UNP A0A0G2JQ44
G	400	HIS	-	expression tag	UNP A0A0G2JQ44
H	395	HIS	-	expression tag	UNP A0A0G2JQ44
H	396	HIS	-	expression tag	UNP A0A0G2JQ44
H	397	HIS	-	expression tag	UNP A0A0G2JQ44
H	398	HIS	-	expression tag	UNP A0A0G2JQ44
H	399	HIS	-	expression tag	UNP A0A0G2JQ44
H	400	HIS	-	expression tag	UNP A0A0G2JQ44

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.

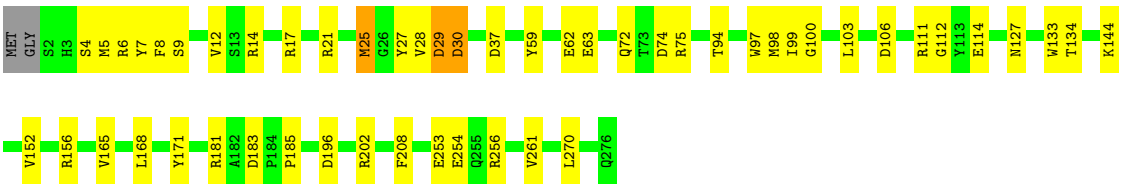
• Molecule 1: HLA class I histocompatibility antigen, alpha chain G

Chain A:



• Molecule 1: HLA class I histocompatibility antigen, alpha chain G

Chain D:

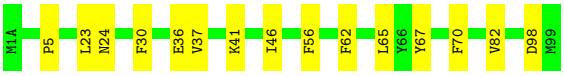


• Molecule 2: Beta-2-microglobulin

Chain B:

• Molecule 2: Beta-2-microglobulin

Chain E:



• Molecule 3: 9 Mer Peptide (RL9) From Histone H2A.x

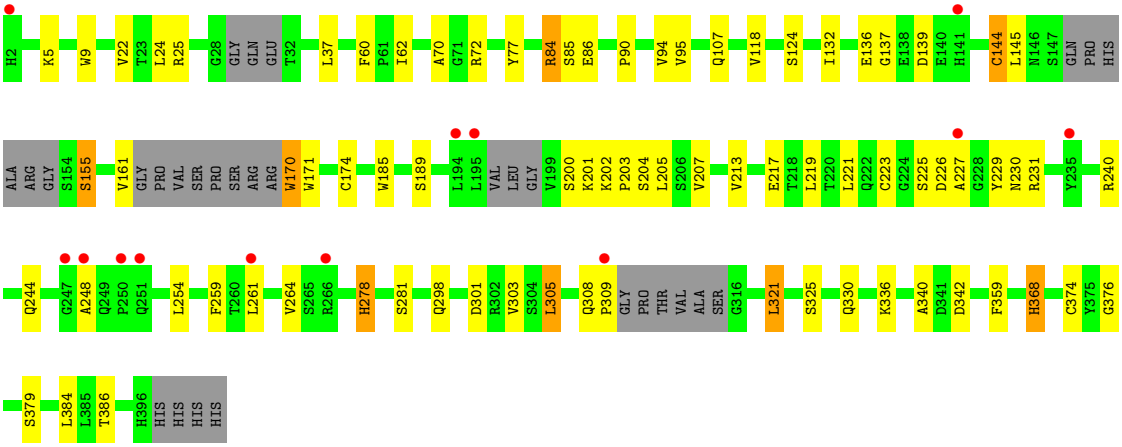
Chain C:

• Molecule 3: 9 Mer Peptide (RL9) From Histone H2A.x

Chain F:

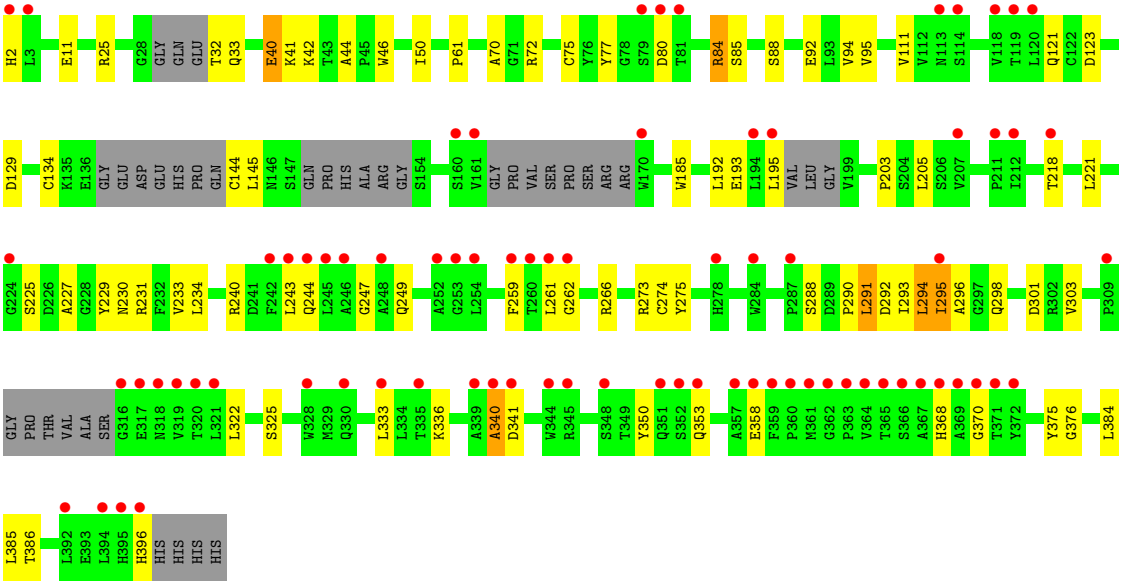
• Molecule 4: Leukocyte immunoglobulin-like receptor subfamily B member 1

Chain G:



• Molecule 4: Leukocyte immunoglobulin-like receptor subfamily B member 1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.68Å 154.68Å 98.20Å 90.00° 102.24° 90.00°	Depositor
Resolution (Å)	45.42 – 3.30 45.42 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (45.42-3.30) 97.8 (45.42-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.220 , 0.267 0.220 , 0.267	Depositor DCC
R_{free} test set	1509 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	66.1	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 25.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	12038	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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	0.23	0/2303	0.44	1/3124 (0.0%)
1	D	0.24	0/2303	0.45	1/3124 (0.0%)
2	B	0.24	0/860	0.42	0/1162
2	E	0.23	0/860	0.42	0/1162
3	C	0.23	0/82	0.36	0/108
3	F	0.22	0/82	0.39	0/108
4	G	0.25	0/2968	0.48	0/4042
4	H	0.25	0/2909	0.49	0/3960
All	All	0.24	0/12367	0.46	2/16790 (0.0%)

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	A	0	2
1	D	0	2
4	G	0	2
4	H	0	3
All	All	0	9

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	28	VAL	C-N-CA	7.13	139.52	121.70
1	D	28	VAL	C-N-CA	6.45	137.83	121.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	ASP	Peptide
1	A	30	ASP	Peptide
1	D	29	ASP	Peptide
1	D	30	ASP	Peptide
4	G	340	ALA	Peptide
4	G	368	HIS	Peptide
4	H	340	ALA	Peptide
4	H	40	GLU	Peptide
4	H	80	ASP	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	A	2242	0	2096	34	0
1	D	2242	0	2096	34	0
2	B	837	0	803	7	0
2	E	837	0	803	9	0
3	C	81	0	94	0	0
3	F	81	0	94	1	0
4	G	2887	0	2748	46	0
4	H	2831	0	2706	60	0
All	All	12038	0	11440	184	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 8.

All (184) 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)
4:H:205:LEU:HD22	4:H:291:LEU:HD12	1.56	0.87
4:H:295:ILE:HD11	4:H:298:GLN:CG	2.08	0.84
4:H:295:ILE:HD12	4:H:296:ALA:N	1.92	0.84
4:G:203:PRO:HA	4:G:225:SER:HB2	1.61	0.80
4:H:295:ILE:HD11	4:H:298:GLN:HG2	1.66	0.76
4:H:294:LEU:HD23	4:H:294:LEU:N	2.01	0.74
4:H:293:ILE:C	4:H:294:LEU:HD23	2.08	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:5:LYS:HB3	4:G:86:GLU:HG3	1.72	0.72
4:H:273:ARG:HH21	4:H:290:PRO:HG3	1.54	0.71
4:H:221:LEU:HB2	4:H:259:PHE:HB2	1.73	0.70
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.72	0.70
4:H:2:HIS:N	4:H:77:TYR:HH	1.88	0.69
4:H:295:ILE:HD11	4:H:298:GLN:HG3	1.75	0.67
4:G:278:HIS:HD1	4:G:281:SER:HG	1.41	0.67
4:H:84:ARG:NH1	4:H:85:SER:O	2.26	0.67
4:H:295:ILE:HD12	4:H:295:ILE:C	2.15	0.67
1:D:4:SER:N	1:D:29:ASP:OD1	2.28	0.66
4:G:124:SER:O	4:G:155:SER:OG	2.14	0.66
4:G:84:ARG:NH1	4:G:85:SER:O	2.29	0.66
1:A:220:ASP:OD2	1:A:256:ARG:NH1	2.31	0.64
4:G:305:LEU:HG	4:G:374:CYS:SG	2.38	0.64
1:A:202:ARG:NH1	2:B:98:ASP:O	2.31	0.64
1:D:12:VAL:HG22	1:D:94:THR:HG23	1.78	0.64
1:A:6:ARG:NH1	1:A:113:TYR:OH	2.32	0.63
4:H:11:GLU:OE2	4:H:25:ARG:NH1	2.32	0.62
4:H:336:LYS:NZ	4:H:368:HIS:O	2.22	0.62
1:D:111:ARG:NH1	1:D:112:GLY:O	2.32	0.62
1:A:55:GLU:OE1	1:A:170:ARG:NH2	2.33	0.61
1:A:181:ARG:NH1	1:A:183:ASP:OD2	2.33	0.61
1:D:261:VAL:HG22	1:D:270:LEU:HB2	1.83	0.61
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.83	0.61
4:H:266:ARG:HG3	4:H:384:LEU:HD21	1.82	0.60
4:G:278:HIS:ND1	4:G:281:SER:OG	2.29	0.60
4:H:32:THR:HG23	4:H:33:GLN:H	1.67	0.60
1:D:181:ARG:NH1	1:D:183:ASP:OD2	2.35	0.60
1:A:191:HIS:NE2	1:A:254:GLU:OE1	2.35	0.59
1:A:103:LEU:HD11	1:A:165:VAL:HG13	1.85	0.59
2:B:56:PHE:HA	2:B:62:PHE:HA	1.86	0.58
1:A:59:TYR:HH	1:A:171:TYR:HH	1.51	0.58
1:A:204:TRP:HE3	1:A:206:LEU:HD21	1.67	0.58
1:D:14:ARG:HB2	1:D:17:ARG:HB2	1.85	0.58
2:B:81:ARG:NH2	2:E:36:GLU:OE2	2.36	0.58
1:D:103:LEU:HD13	1:D:168:LEU:HD23	1.86	0.56
1:D:59:TYR:HH	1:D:171:TYR:HH	1.53	0.56
4:H:376:GLY:H	4:H:386:THR:HG22	1.70	0.56
4:G:139:ASP:N	4:G:139:ASP:OD1	2.37	0.56
1:D:103:LEU:HD11	1:D:165:VAL:HG13	1.87	0.55
4:H:218:THR:HG23	4:H:262:GLY:HA2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:155:SER:OG	4:G:155:SER:O	2.21	0.55
4:H:322:LEU:HD12	4:H:358:GLU:HG2	1.89	0.55
4:G:70:ALA:HB2	4:G:95:VAL:HG23	1.87	0.55
4:H:129:ASP:OD1	4:H:129:ASP:N	2.39	0.55
1:A:12:VAL:HG22	1:A:94:THR:HG23	1.89	0.55
1:D:9:SER:HB3	1:D:97:TRP:HB3	1.88	0.55
4:H:333:LEU:HB2	4:H:375:TYR:HB2	1.88	0.54
4:H:303:VAL:HG12	4:H:325:SER:HB3	1.89	0.54
1:D:7:TYR:HB2	1:D:99:ILE:HG22	1.90	0.54
4:G:303:VAL:HG12	4:G:325:SER:HB2	1.90	0.53
4:H:301:ASP:N	4:H:301:ASP:OD1	2.38	0.53
1:D:25:MET:N	1:D:25:MET:SD	2.81	0.53
4:H:244:GLN:HB2	4:H:259:PHE:CD1	2.44	0.53
1:D:62:GLU:OE1	3:F:1:ARG:NH1	2.42	0.53
4:H:72:ARG:HG2	4:H:92:GLU:HG2	1.90	0.53
4:G:94:VAL:HG11	4:G:185:TRP:CD2	2.44	0.52
4:G:230:ASN:O	4:G:248:ALA:N	2.43	0.52
4:H:274:CYS:O	4:H:288:SER:OG	2.27	0.52
4:G:330:GLN:HG3	4:G:379:SER:H	1.72	0.52
4:G:219:LEU:HD23	4:G:264:VAL:HG11	1.90	0.52
4:H:340:ALA:O	4:H:341:ASP:OD2	2.28	0.51
4:G:132:ILE:HG22	4:G:144:CYS:SG	2.50	0.51
4:H:70:ALA:HB2	4:H:95:VAL:HG23	1.92	0.51
4:H:111:VAL:HG22	4:H:195:LEU:HD12	1.90	0.51
4:H:221:LEU:HD13	4:H:261:LEU:HD13	1.92	0.51
1:A:45:MET:HG2	1:A:63:GLU:HB3	1.92	0.51
4:G:118:VAL:HG12	4:G:161:VAL:HG22	1.92	0.51
4:H:50:ILE:HD12	4:H:61:PRO:HD2	1.91	0.51
4:H:336:LYS:HE3	4:H:370:GLY:HA3	1.93	0.51
4:G:9:TRP:CZ2	4:G:25:ARG:HG2	2.47	0.50
1:D:254:GLU:OE1	1:D:254:GLU:N	2.44	0.50
4:G:226:ASP:HA	4:G:254:LEU:HA	1.94	0.50
4:G:301:ASP:OD1	4:G:301:ASP:N	2.45	0.49
1:D:6:ARG:HD3	1:D:100:GLY:HA3	1.94	0.49
4:G:136:GLU:N	4:G:171:TRP:O	2.45	0.49
4:H:40:GLU:O	4:H:42:LYS:N	2.45	0.49
4:G:136:GLU:HG2	4:G:137:GLY:H	1.78	0.49
2:E:37:VAL:HG22	2:E:82:VAL:HG22	1.95	0.49
4:H:94:VAL:HG11	4:H:185:TRP:CD2	2.48	0.49
1:A:25:MET:SD	1:A:25:MET:N	2.86	0.49
1:A:4:SER:N	1:A:29:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:GLU:OE2	1:D:156:ARG:NH2	2.32	0.48
4:G:94:VAL:HG11	4:G:185:TRP:CE2	2.48	0.48
1:D:253:GLU:OE1	1:D:256:ARG:NH2	2.46	0.48
2:E:5:PRO:HB3	2:E:30:PHE:HB3	1.95	0.48
1:D:133:TRP:HB2	1:D:144:LYS:HG3	1.96	0.48
4:G:22:VAL:HG12	4:G:62:ILE:HB	1.96	0.47
1:A:202:ARG:HE	1:A:246:ALA:HB2	1.79	0.47
4:H:294:LEU:N	4:H:294:LEU:CD2	2.73	0.47
4:H:121:GLN:NE2	4:H:123:ASP:OD2	2.32	0.47
1:A:9:SER:HB3	1:A:97:TRP:HE3	1.79	0.47
1:D:127:ASN:OD1	1:D:134:THR:OG1	2.23	0.47
4:G:213:VAL:HG23	4:G:217:GLU:HB3	1.96	0.47
4:G:230:ASN:OD1	4:G:231:ARG:N	2.48	0.47
2:E:41:LYS:HB2	2:E:46:ILE:HD11	1.96	0.46
4:G:72:ARG:HH21	4:G:90:PRO:HG3	1.80	0.46
4:G:207:VAL:HB	4:G:221:LEU:HD23	1.97	0.46
4:G:376:GLY:H	4:G:386:THR:HG22	1.80	0.46
4:G:336:LYS:NZ	4:G:368:HIS:O	2.42	0.46
1:A:63:GLU:O	1:A:67:THR:OG1	2.30	0.46
4:G:321:LEU:HD12	4:G:359:PHE:HB2	1.97	0.46
4:H:350:TYR:CZ	4:H:353:GLN:HA	2.51	0.46
4:H:203:PRO:HA	4:H:225:SER:HB2	1.97	0.46
1:A:137:ASP:OD1	1:A:137:ASP:N	2.49	0.46
2:B:23:LEU:O	2:B:67:TYR:HA	2.16	0.46
4:H:294:LEU:O	4:H:295:ILE:HG22	2.16	0.46
1:D:98:MET:O	1:D:114:GLU:HA	2.16	0.45
1:D:59:TYR:O	1:D:63:GLU:HG2	2.16	0.45
4:G:24:LEU:HB2	4:G:60:PHE:HB2	1.98	0.45
4:H:94:VAL:HG11	4:H:185:TRP:CE2	2.52	0.45
1:D:8:PHE:HB2	1:D:25:MET:SD	2.56	0.45
2:E:23:LEU:O	2:E:67:TYR:HA	2.16	0.45
4:G:24:LEU:HD13	4:G:37:LEU:HD21	1.99	0.45
4:H:230:ASN:O	4:H:247:GLY:HA2	2.16	0.45
4:H:230:ASN:OD1	4:H:231:ARG:N	2.49	0.45
1:D:253:GLU:HB3	1:D:256:ARG:HD3	1.98	0.45
1:A:103:LEU:HD13	1:A:168:LEU:HD23	1.98	0.44
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.99	0.44
2:E:56:PHE:HA	2:E:62:PHE:HA	1.99	0.44
4:G:174:CYS:N	4:G:189:SER:OG	2.44	0.44
4:H:234:LEU:HG	4:H:243:LEU:HD12	1.99	0.44
4:G:204:SER:O	4:G:223:CYS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:PHE:CE2	1:A:198:GLU:HB2	2.52	0.44
1:D:196:ASP:N	1:D:196:ASP:OD1	2.51	0.44
4:H:192:LEU:HD12	4:H:240:ARG:HD3	2.00	0.44
1:A:14:ARG:HB2	1:A:17:ARG:HB2	1.99	0.43
1:D:27:TYR:HD2	1:D:30:ASP:O	2.01	0.43
1:A:82:ARG:NH1	1:A:89:GLU:HG2	2.33	0.43
1:A:234:ARG:NH1	2:B:8:GLN:OE1	2.51	0.43
1:D:152:VAL:O	1:D:156:ARG:HG2	2.18	0.43
1:D:202:ARG:NH1	2:E:98:ASP:O	2.39	0.43
4:H:75:CYS:N	4:H:88:SER:OG	2.48	0.43
1:A:207:GLY:HA2	1:A:240:THR:HB	2.01	0.43
1:D:106:ASP:OD1	1:D:106:ASP:N	2.51	0.43
4:H:295:ILE:CD1	4:H:298:GLN:HG2	2.42	0.43
1:A:27:TYR:HD2	1:A:30:ASP:O	2.02	0.43
4:H:44:ALA:HB1	4:H:46:TRP:CD1	2.54	0.43
4:G:298:GLN:HG3	4:G:384:LEU:HG	1.99	0.42
1:A:9:SER:OG	1:A:97:TRP:HB3	2.20	0.42
1:D:9:SER:HB3	1:D:97:TRP:HE3	1.84	0.42
1:D:72:GLN:OE1	1:D:75:ARG:NH1	2.53	0.42
4:G:308:GLN:HB2	4:G:309:PRO:HD3	2.00	0.42
2:E:24:ASN:HB3	2:E:65:LEU:HD11	2.01	0.42
4:G:227:ALA:HB3	4:G:229:TYR:CE2	2.55	0.42
4:G:244:GLN:OE1	4:G:259:PHE:HA	2.20	0.42
4:H:42:LYS:HB3	4:H:42:LYS:NZ	2.34	0.42
1:A:219:ARG:HD3	1:A:256:ARG:HH22	1.84	0.42
4:H:295:ILE:O	4:H:385:LEU:HB2	2.20	0.42
1:A:36:PHE:HB2	1:A:45:MET:SD	2.59	0.42
4:H:233:VAL:HG12	4:H:275:TYR:HB2	2.00	0.41
1:A:121:LYS:HE2	1:A:121:LYS:HB3	1.74	0.41
4:G:132:ILE:CG2	4:G:144:CYS:SG	3.09	0.41
4:G:107:GLN:OE1	4:G:240:ARG:NH2	2.30	0.41
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.03	0.41
4:H:227:ALA:HB3	4:H:229:TYR:CZ	2.55	0.41
4:H:295:ILE:HD12	4:H:296:ALA:CA	2.51	0.41
1:A:71:ALA:O	1:A:75:ARG:HG3	2.21	0.41
1:D:185:PRO:HB3	1:D:208:PHE:HB3	2.03	0.41
1:A:59:TYR:OH	1:A:171:TYR:OH	2.24	0.41
1:A:197:TYR:CE2	4:G:84:ARG:HD3	2.56	0.41
1:D:8:PHE:HB3	2:E:56:PHE:CZ	2.56	0.41
4:G:170:TRP:HB3	4:G:171:TRP:CD1	2.56	0.41
4:H:205:LEU:HD21	4:H:221:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:244:GLN:HB2	4:H:259:PHE:HD1	1.83	0.41
4:H:295:ILE:CD1	4:H:296:ALA:N	2.73	0.41
4:H:205:LEU:HD12	4:H:274:CYS:N	2.36	0.41
4:G:202:LYS:HA	4:G:203:PRO:HD3	1.96	0.40
1:A:195:PHE:HE2	1:A:198:GLU:HB2	1.86	0.40
4:H:291:LEU:HD23	4:H:291:LEU:HA	1.71	0.40
4:G:200:SER:OG	4:G:201:LYS:N	2.55	0.40
4:H:193:GLU:H	4:H:240:ARG:NH1	2.20	0.40
1:D:21:ARG:NH2	1:D:37:ASP:OD2	2.55	0.40
4:H:134:CYS:HA	4:H:144:CYS:HA	2.04	0.40
1:A:230:LEU:HD12	1:A:245:ALA:HB2	2.04	0.40
4:G:219:LEU:HD11	4:G:261:LEU:HD22	2.03	0.40
4:H:294:LEU:C	4:H:295:ILE:CG2	2.89	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	273/277 (99%)	272 (100%)	1 (0%)	0	100	100
1	D	273/277 (99%)	272 (100%)	1 (0%)	0	100	100
2	B	98/100 (98%)	98 (100%)	0	0	100	100
2	E	98/100 (98%)	98 (100%)	0	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
4	G	357/399 (90%)	357 (100%)	0	0	100	100
4	H	348/399 (87%)	345 (99%)	3 (1%)	0	100	100
All	All	1461/1570 (93%)	1456 (100%)	5 (0%)	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	232/233 (100%)	224 (97%)	8 (3%)	37 65
1	D	232/233 (100%)	230 (99%)	2 (1%)	78 87
2	B	95/95 (100%)	93 (98%)	2 (2%)	53 75
2	E	95/95 (100%)	94 (99%)	1 (1%)	73 85
3	C	9/9 (100%)	8 (89%)	1 (11%)	6 23
3	F	9/9 (100%)	8 (89%)	1 (11%)	6 23
4	G	316/340 (93%)	305 (96%)	11 (4%)	36 64
4	H	310/340 (91%)	301 (97%)	9 (3%)	42 69
All	All	1298/1354 (96%)	1263 (97%)	35 (3%)	44 71

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	25	MET
1	A	45	MET
1	A	74	ASP
1	A	113	TYR
1	A	195	PHE
1	A	234	ARG
1	A	270	LEU
2	B	64	LEU
2	B	70	PHE
3	C	5	ARG
1	D	25	MET
1	D	74	ASP
2	E	70	PHE
3	F	1	ARG
4	G	77	TYR

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Mol	Chain	Res	Type
4	G	84	ARG
4	G	144	CYS
4	G	145	LEU
4	G	155	SER
4	G	170	TRP
4	G	205	LEU
4	G	278	HIS
4	G	305	LEU
4	G	321	LEU
4	G	342	ASP
4	H	41	LYS
4	H	84	ARG
4	H	145	LEU
4	H	249	GLN
4	H	291	LEU
4	H	292	ASP
4	H	294	LEU
4	H	295	ILE
4	H	396	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	HIS

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)

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	A	275/277 (99%)	-0.24	0 100 100	36, 55, 77, 91	0
1	D	275/277 (99%)	-0.17	0 100 100	32, 52, 77, 91	0
2	B	100/100 (100%)	-0.21	0 100 100	31, 50, 72, 81	0
2	E	100/100 (100%)	-0.16	0 100 100	39, 52, 70, 75	0
3	C	9/9 (100%)	0.06	0 100 100	44, 47, 61, 64	0
3	F	9/9 (100%)	0.00	0 100 100	46, 50, 58, 74	0
4	G	369/399 (92%)	0.20	13 (3%) 44 42	38, 73, 127, 167	0
4	H	362/399 (90%)	0.97	77 (21%) 0 1	51, 116, 169, 181	0
All	All	1499/1570 (95%)	0.18	90 (6%) 21 21	31, 63, 148, 181	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	244	GLN	6.9
4	H	309	PRO	6.6
4	H	372	TYR	6.5
4	H	260	THR	6.5
4	H	2	HIS	6.3
4	H	366	SER	5.8
4	H	170	TRP	5.8
4	G	251	GLN	5.7
4	H	320	THR	5.7
4	H	361	MET	5.6
4	H	319	VAL	5.5
4	H	365	THR	5.3
4	H	252	ALA	5.1
4	H	3	LEU	5.1
4	G	309	PRO	5.0
4	H	367	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
4	H	321	LEU	4.7
4	H	245	LEU	4.7
4	H	394	LEU	4.6
4	H	392	LEU	4.4
4	H	261	LEU	4.4
4	H	194	LEU	4.3
4	H	316	GLY	4.3
4	G	2	HIS	4.3
4	H	318	ASN	4.2
4	H	253	GLY	4.1
4	H	340	ALA	4.1
4	H	243	LEU	4.0
4	H	351	GLN	3.9
4	H	242	PHE	3.9
4	G	194	LEU	3.8
4	H	359	PHE	3.8
4	H	218	THR	3.7
4	H	339	ALA	3.6
4	G	261	LEU	3.6
4	H	396	HIS	3.6
4	H	370	GLY	3.6
4	H	81	THR	3.4
4	H	317	GLU	3.3
4	H	395	HIS	3.2
4	H	212	ILE	3.2
4	H	262	GLY	3.1
4	H	353	GLN	3.1
4	G	248	ALA	3.1
4	H	360	PRO	3.0
4	H	341	ASP	3.0
4	H	246	ALA	3.0
4	H	113	ASN	3.0
4	H	358	GLU	3.0
4	H	114	SER	3.0
4	H	357	ALA	2.9
4	H	369	ALA	2.9
4	H	248	ALA	2.9
4	H	344	TRP	2.8
4	H	368	HIS	2.8
4	H	254	LEU	2.7
4	H	330	GLN	2.7
4	H	284	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
4	H	363	PRO	2.6
4	G	250	PRO	2.6
4	G	141	HIS	2.6
4	H	335	THR	2.6
4	H	364	VAL	2.6
4	H	345	ARG	2.6
4	H	362	GLY	2.5
4	H	328	TRP	2.5
4	G	235	TYR	2.5
4	G	247	GLY	2.5
4	H	278	HIS	2.5
4	H	207	VAL	2.5
4	H	120	LEU	2.5
4	H	195	LEU	2.4
4	H	79	SER	2.4
4	H	80	ASP	2.4
4	G	227	ALA	2.4
4	H	352	SER	2.4
4	H	211	PRO	2.3
4	G	266	ARG	2.3
4	H	118	VAL	2.3
4	H	160	SER	2.2
4	H	224	GLY	2.2
4	H	371	THR	2.2
4	H	259	PHE	2.2
4	H	119	THR	2.1
4	H	161	VAL	2.1
4	H	295	ILE	2.1
4	H	348	SER	2.1
4	G	195	LEU	2.0
4	H	287	PRO	2.0
4	H	333	LEU	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.