Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 08:52 PM GMT

PDB ID	:	4YHD
Title	:	Staphylococcal alpha-hemolysin H35A mutant monomer
Authors	:	Sugawara, T.; Kato, K.; Tanaka, Y.; Yao, M.
Deposited on	:	2015-02-27
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

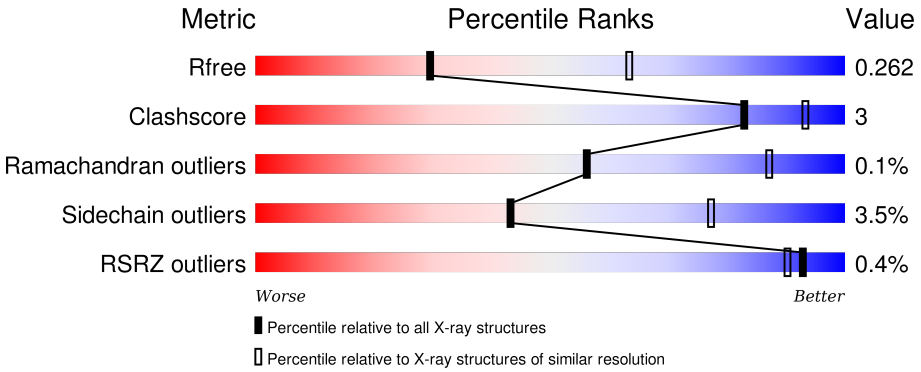
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	302	82% 11% 7%
1	B	302	85% 8% • 6%
1	C	302	% 84% 8% 8%
1	D	302	85% 6% • 7%
1	E	302	% 75% 12% • 11%

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Mol	Chain	Length	Quality of chain
1	G	302	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26567 atoms, of which 13065 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 Alpha-hemolysin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	281	Total	C	H	N	O	S	0	0	0
			4458	1426	2193	386	446	7			
1	B	283	Total	C	H	N	O	S	0	0	0
			4483	1437	2199	393	447	7			
1	C	279	Total	C	H	N	O	S	0	0	0
			4429	1417	2185	382	438	7			
1	D	282	Total	C	H	N	O	S	0	0	0
			4472	1430	2200	387	448	7			
1	E	268	Total	C	H	N	O	S	0	0	0
			4266	1366	2098	366	429	7			
1	G	281	Total	C	H	N	O	S	0	0	0
			4454	1424	2190	386	447	7			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P09616
A	35	ALA	HIS	engineered mutation	UNP P09616
A	208	GLU	ASP	engineered mutation	UNP P09616
A	294	LEU	-	expression tag	UNP P09616
A	295	GLU	-	expression tag	UNP P09616
A	296	HIS	-	expression tag	UNP P09616
A	297	HIS	-	expression tag	UNP P09616
A	298	HIS	-	expression tag	UNP P09616
A	299	HIS	-	expression tag	UNP P09616
A	300	HIS	-	expression tag	UNP P09616
A	301	HIS	-	expression tag	UNP P09616
B	0	MET	-	initiating methionine	UNP P09616
B	35	ALA	HIS	engineered mutation	UNP P09616
B	208	GLU	ASP	engineered mutation	UNP P09616
B	294	LEU	-	expression tag	UNP P09616
B	295	GLU	-	expression tag	UNP P09616
B	296	HIS	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
B	297	HIS	-	expression tag	UNP P09616
B	298	HIS	-	expression tag	UNP P09616
B	299	HIS	-	expression tag	UNP P09616
B	300	HIS	-	expression tag	UNP P09616
B	301	HIS	-	expression tag	UNP P09616
C	0	MET	-	initiating methionine	UNP P09616
C	35	ALA	HIS	engineered mutation	UNP P09616
C	208	GLU	ASP	engineered mutation	UNP P09616
C	294	LEU	-	expression tag	UNP P09616
C	295	GLU	-	expression tag	UNP P09616
C	296	HIS	-	expression tag	UNP P09616
C	297	HIS	-	expression tag	UNP P09616
C	298	HIS	-	expression tag	UNP P09616
C	299	HIS	-	expression tag	UNP P09616
C	300	HIS	-	expression tag	UNP P09616
C	301	HIS	-	expression tag	UNP P09616
D	0	MET	-	initiating methionine	UNP P09616
D	35	ALA	HIS	engineered mutation	UNP P09616
D	208	GLU	ASP	engineered mutation	UNP P09616
D	294	LEU	-	expression tag	UNP P09616
D	295	GLU	-	expression tag	UNP P09616
D	296	HIS	-	expression tag	UNP P09616
D	297	HIS	-	expression tag	UNP P09616
D	298	HIS	-	expression tag	UNP P09616
D	299	HIS	-	expression tag	UNP P09616
D	300	HIS	-	expression tag	UNP P09616
D	301	HIS	-	expression tag	UNP P09616
E	0	MET	-	initiating methionine	UNP P09616
E	35	ALA	HIS	engineered mutation	UNP P09616
E	208	GLU	ASP	engineered mutation	UNP P09616
E	294	LEU	-	expression tag	UNP P09616
E	295	GLU	-	expression tag	UNP P09616
E	296	HIS	-	expression tag	UNP P09616
E	297	HIS	-	expression tag	UNP P09616
E	298	HIS	-	expression tag	UNP P09616
E	299	HIS	-	expression tag	UNP P09616
E	300	HIS	-	expression tag	UNP P09616
E	301	HIS	-	expression tag	UNP P09616
G	0	MET	-	initiating methionine	UNP P09616
G	35	ALA	HIS	engineered mutation	UNP P09616
G	208	GLU	ASP	engineered mutation	UNP P09616
G	294	LEU	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
G	295	GLU	-	expression tag	UNP P09616
G	296	HIS	-	expression tag	UNP P09616
G	297	HIS	-	expression tag	UNP P09616
G	298	HIS	-	expression tag	UNP P09616
G	299	HIS	-	expression tag	UNP P09616
G	300	HIS	-	expression tag	UNP P09616
G	301	HIS	-	expression tag	UNP P09616

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

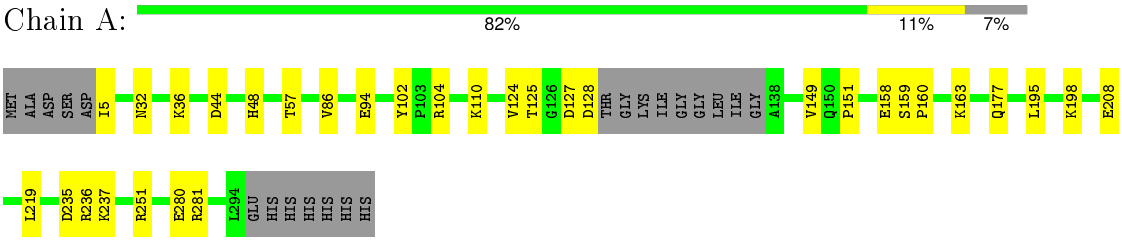
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

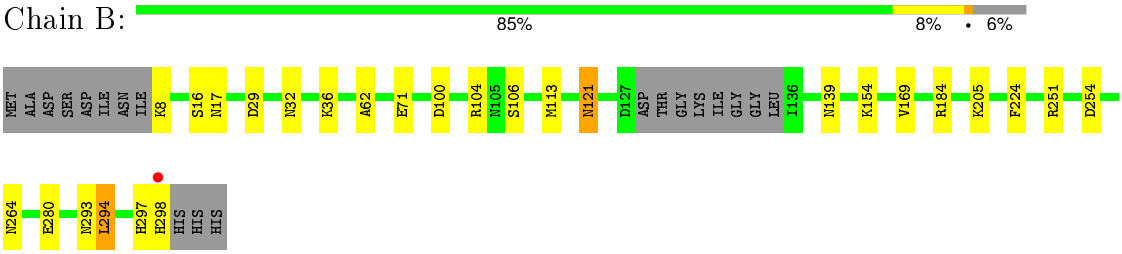
- Molecule 1: Alpha-hemolysin

Chain A:



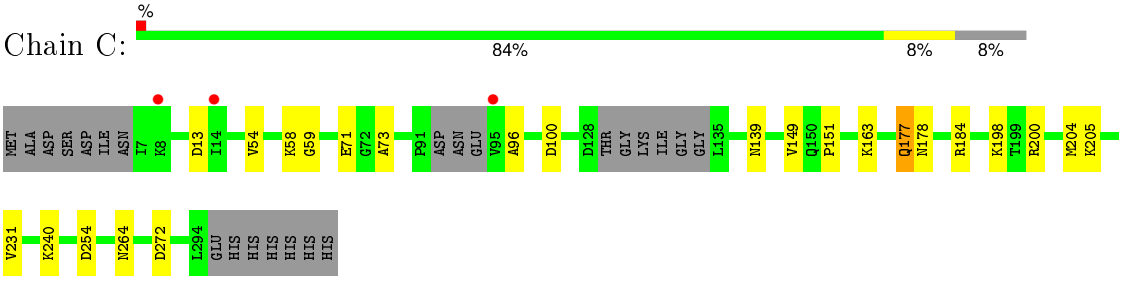
- Molecule 1: Alpha-hemolysin

Chain B:



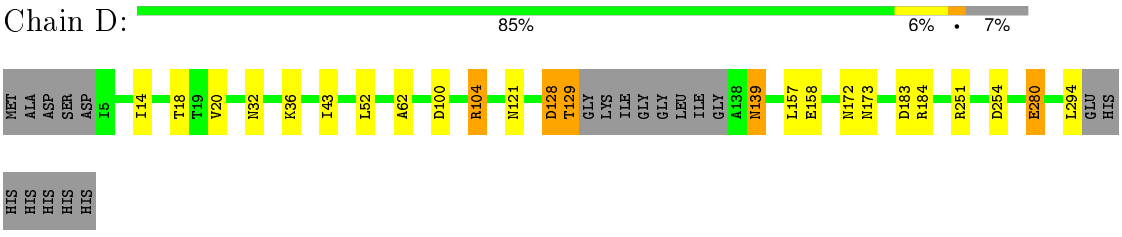
- Molecule 1: Alpha-hemolysin

Chain C:



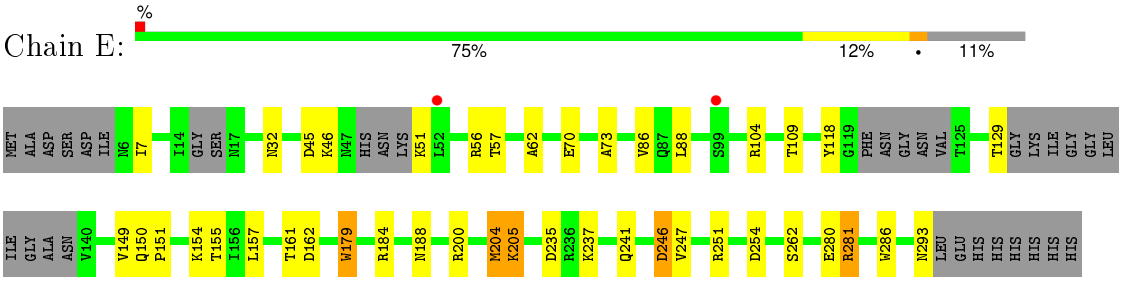
- Molecule 1: Alpha-hemolysin

Chain D:



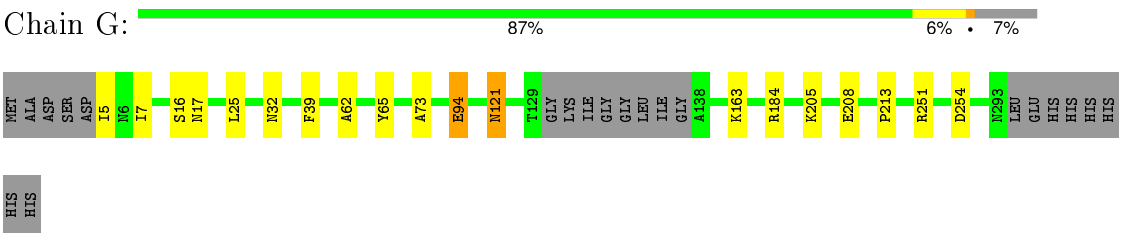
• Molecule 1: Alpha-hemolysin

Chain E:



• Molecule 1: Alpha-hemolysin

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.93Å 128.91Å 135.28Å 90.00° 91.57° 90.00°	Depositor
Resolution (Å)	37.39 – 2.80 49.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.8 (37.39-2.80) 95.8 (49.13-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.215 , 0.263 0.215 , 0.262	Depositor DCC
R_{free} test set	3070 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 8.4	EDS
Estimated twinning fraction	0.014 for -h,l,k 0.019 for -h,-l,-k 0.058 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 61440 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	26567	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CL

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	0.25	0/2315	0.43	0/3133
1	B	0.27	0/2337	0.44	0/3162
1	C	0.24	0/2293	0.43	0/3101
1	D	0.24	0/2322	0.43	0/3143
1	E	0.25	0/2213	0.42	0/2991
1	G	0.25	0/2314	0.44	0/3132
All	All	0.25	0/13794	0.43	0/18662

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	2265	2193	2194	18	0
1	B	2284	2199	2203	13	0
1	C	2244	2185	2185	9	0
1	D	2272	2200	2201	12	0
1	E	2168	2098	2098	21	0
1	G	2264	2190	2190	11	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	1	0
2	G	1	0	0	0	0
All	All	13502	13065	13071	82	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 3.

All (82) 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:70:GLU:OE2	1:E:205:LYS:NZ	1.83	1.10
1:A:198:LYS:NZ	1:A:208:GLU:O	2.06	0.86
1:G:94:GLU:O	1:G:163:LYS:NZ	2.12	0.83
1:C:177:GLN:NE2	1:C:198:LYS:O	2.15	0.80
1:B:113:MET:SD	1:E:237:LYS:NZ	2.53	0.78
1:C:96:ALA:O	1:C:163:LYS:NZ	2.17	0.77
1:G:205:LYS:NZ	1:G:208:GLU:OE1	2.18	0.76
1:E:51:LYS:NZ	1:E:286:TRP:O	2.19	0.76
1:A:44:ASP:OD1	1:A:236:ARG:NH2	2.23	0.71
1:A:177:GLN:NE2	1:A:198:LYS:O	2.25	0.69
1:E:32:ASN:O	1:E:251:ARG:NH2	2.27	0.68
1:G:32:ASN:O	1:G:251:ARG:NH2	2.27	0.67
1:E:246:ASP:OD1	1:E:281:ARG:NH1	2.28	0.67
1:G:62:ALA:O	1:G:251:ARG:NH1	2.29	0.65
1:D:62:ALA:O	1:D:251:ARG:NH1	2.28	0.65
1:B:100:ASP:OD1	1:B:104:ARG:NH2	2.32	0.63
1:B:62:ALA:O	1:B:251:ARG:NH1	2.31	0.63
1:C:149:VAL:HG13	1:C:151:PRO:HD3	1.83	0.60
1:E:57:THR:HG21	1:E:86:VAL:HG11	1.84	0.59
1:D:32:ASN:O	1:D:251:ARG:NH2	2.33	0.59
1:G:16:SER:OG	1:G:17:ASN:N	2.36	0.58
1:E:62:ALA:O	1:E:251:ARG:NH1	2.37	0.57
1:D:100:ASP:OD1	1:D:104:ARG:NH1	2.38	0.56
1:E:45:ASP:OD1	1:E:46:LYS:N	2.38	0.56
1:A:151:PRO:HD2	1:A:219:LEU:HD13	1.89	0.55
1:B:169:VAL:HG21	1:B:224:PHE:CZ	2.41	0.55
1:E:188:ASN:ND2	2:E:401:CL:CL	2.67	0.55
1:A:128:ASP:OD1	1:A:128:ASP:N	2.39	0.55
1:G:5:ILE:HG23	1:G:7:ILE:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ASN:O	1:A:251:ARG:NH2	2.40	0.53
1:B:32:ASN:O	1:B:251:ARG:NH2	2.39	0.52
1:E:235:ASP:O	1:E:241:GLN:NE2	2.41	0.52
1:B:113:MET:CE	1:E:237:LYS:HZ1	2.23	0.52
1:D:128:ASP:N	1:D:128:ASP:OD1	2.43	0.52
1:A:149:VAL:HG12	1:A:151:PRO:HD3	1.91	0.51
1:A:94:GLU:O	1:A:163:LYS:NZ	2.45	0.50
1:G:121:ASN:OD1	1:G:121:ASN:N	2.45	0.49
1:C:184:ARG:HD2	1:C:254:ASP:OD2	2.13	0.49
1:B:71:GLU:N	1:B:71:GLU:OE1	2.47	0.48
1:B:293:ASN:OD1	1:B:294:LEU:N	2.47	0.48
1:E:88:LEU:HG	1:E:247:VAL:HG13	1.97	0.47
1:G:7:ILE:HG21	1:G:39:PHE:CD1	2.50	0.47
1:A:48:HIS:O	1:A:236:ARG:NH1	2.48	0.47
1:D:43:ILE:HB	1:D:52:LEU:HB2	1.96	0.46
1:A:36:LYS:NZ	1:A:280:GLU:HG2	2.31	0.46
1:B:184:ARG:HD2	1:B:254:ASP:OD2	2.16	0.46
1:C:58:LYS:HG2	1:C:59:GLY:H	1.80	0.46
1:E:149:VAL:HG12	1:E:151:PRO:HD3	1.98	0.45
1:C:71:GLU:N	1:C:71:GLU:OE1	2.49	0.45
1:B:36:LYS:HZ1	1:B:280:GLU:HG2	1.80	0.45
1:B:121:ASN:OD1	1:B:121:ASN:N	2.48	0.45
1:E:45:ASP:OD2	1:E:118:TYR:OH	2.29	0.45
1:D:14:ILE:HG12	1:D:20:VAL:HG23	1.97	0.45
1:A:36:LYS:HZ1	1:A:280:GLU:HG2	1.82	0.45
1:D:139:ASN:N	1:D:139:ASN:OD1	2.50	0.45
1:E:162:ASP:N	1:E:162:ASP:OD1	2.49	0.45
1:E:7:ILE:HG12	1:E:56:ARG:NH1	2.32	0.44
1:A:102:TYR:OH	1:A:124:VAL:O	2.35	0.44
1:D:100:ASP:CG	1:D:104:ARG:NH1	2.71	0.44
1:G:65:TYR:CD2	1:G:213:PRO:HG3	2.52	0.43
1:A:57:THR:HG21	1:A:86:VAL:HG11	2.00	0.43
1:A:110:LYS:CD	1:A:151:PRO:HA	2.48	0.43
1:D:128:ASP:HA	1:D:129:THR:HB	2.00	0.43
1:E:150:GLN:OE1	1:E:155:THR:OG1	2.33	0.43
1:C:54:VAL:HG13	1:C:231:VAL:HG12	2.00	0.43
1:G:73:ALA:HB1	1:G:205:LYS:HB3	2.01	0.42
1:E:73:ALA:HB1	1:E:205:LYS:HB3	2.01	0.42
1:A:110:LYS:HD3	1:A:151:PRO:HA	2.01	0.42
1:B:297:HIS:O	1:B:298:HIS:HB2	2.19	0.42
1:D:184:ARG:HD2	1:D:254:ASP:OD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:LYS:NZ	1:D:280:GLU:HB2	2.35	0.42
1:E:179:TRP:N	1:E:179:TRP:CD1	2.88	0.42
1:A:235:ASP:OD2	1:A:237:LYS:CG	2.68	0.42
1:G:184:ARG:HD2	1:G:254:ASP:OD2	2.20	0.41
1:D:172:ASN:OD1	1:D:173:ASN:ND2	2.54	0.41
1:A:159:SER:N	1:A:160:PRO:HD3	2.35	0.41
1:E:161:THR:HG22	1:E:162:ASP:N	2.35	0.41
1:A:235:ASP:OD2	1:A:237:LYS:HG2	2.20	0.41
1:B:29:ASP:OD2	1:B:298:HIS:HB3	2.21	0.40
1:C:272:ASP:N	1:C:272:ASP:OD1	2.51	0.40
1:E:184:ARG:HD2	1:E:254:ASP:OD2	2.22	0.40
1:C:73:ALA:HA	1:C:205:LYS:HG3	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	277/302 (92%)	268 (97%)	9 (3%)	0	100	100
1	B	279/302 (92%)	269 (96%)	9 (3%)	1 (0%)	39	74
1	C	273/302 (90%)	263 (96%)	10 (4%)	0	100	100
1	D	278/302 (92%)	265 (95%)	13 (5%)	0	100	100
1	E	258/302 (85%)	242 (94%)	15 (6%)	1 (0%)	39	74
1	G	277/302 (92%)	262 (95%)	15 (5%)	0	100	100
All	All	1642/1812 (91%)	1569 (96%)	71 (4%)	2 (0%)	56	87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	204	MET

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Mol	Chain	Res	Type
1	B	16	SER

5.3.2 Protein sidechains

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	251/267 (94%)	244 (97%)	7 (3%)	51 84
1	B	252/267 (94%)	243 (96%)	9 (4%)	42 76
1	C	248/267 (93%)	239 (96%)	9 (4%)	42 76
1	D	252/267 (94%)	241 (96%)	11 (4%)	35 69
1	E	241/267 (90%)	227 (94%)	14 (6%)	25 57
1	G	251/267 (94%)	248 (99%)	3 (1%)	78 95
All	All	1495/1602 (93%)	1442 (96%)	53 (4%)	43 77

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	104	ARG
1	A	125	THR
1	A	127	ASP
1	A	158	GLU
1	A	195	LEU
1	A	281	ARG
1	B	8	LYS
1	B	17	ASN
1	B	106	SER
1	B	121	ASN
1	B	139	ASN
1	B	154	LYS
1	B	205	LYS
1	B	264	ASN
1	B	294	LEU
1	C	13	ASP

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Mol	Chain	Res	Type
1	C	100	ASP
1	C	139	ASN
1	C	177	GLN
1	C	178	ASN
1	C	200	ARG
1	C	204	MET
1	C	240	LYS
1	C	264	ASN
1	D	18	THR
1	D	104	ARG
1	D	121	ASN
1	D	128	ASP
1	D	129	THR
1	D	139	ASN
1	D	157	LEU
1	D	158	GLU
1	D	183	ASP
1	D	280	GLU
1	D	294	LEU
1	E	104	ARG
1	E	109	THR
1	E	129	THR
1	E	154	LYS
1	E	157	LEU
1	E	179	TRP
1	E	200	ARG
1	E	204	MET
1	E	205	LYS
1	E	246	ASP
1	E	262	SER
1	E	280	GLU
1	E	281	ARG
1	E	293	ASN
1	G	25	LEU
1	G	94	GLU
1	G	121	ASN

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

Mol	Chain	Res	Type
1	C	177	GLN
1	D	173	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 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

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	281/302 (93%)	-0.11	0 100 100	19, 33, 56, 74	0
1	B	283/302 (93%)	-0.09	1 (0%) 93 90	22, 34, 59, 94	0
1	C	279/302 (92%)	-0.10	3 (1%) 82 74	20, 40, 71, 89	0
1	D	282/302 (93%)	-0.13	0 100 100	21, 35, 62, 81	0
1	E	268/302 (88%)	0.13	2 (0%) 89 84	24, 46, 81, 100	0
1	G	281/302 (93%)	-0.10	0 100 100	18, 34, 57, 73	0
All	All	1674/1812 (92%)	-0.07	6 (0%) 93 90	18, 37, 68, 100	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	HIS	3.7
1	C	14	ILE	2.5
1	E	99	SER	2.4
1	C	8	LYS	2.3
1	E	52	LEU	2.2
1	C	95	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	CL	D	401	1/1	0.99	0.26	-	32,32,32,32	0
2	CL	E	401	1/1	0.93	0.18	-	41,41,41,41	0
2	CL	G	401	1/1	0.99	0.20	-	32,32,32,32	0
2	CL	A	401	1/1	0.98	0.28	-	33,33,33,33	0
2	CL	B	401	1/1	0.99	0.29	-	31,31,31,31	0

6.5 Other polymers

There are no such residues in this entry.