Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 11:18 AM JST

PDB ID	:	5X0N
Title	:	Regulatory domain of variant C227S AphB from Vibrio vulnificus
Authors	:	Song, S.; Park, N.; Ha, N.-C.
Deposited on	:	2017-01-22
Resolution	:	2.99 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:

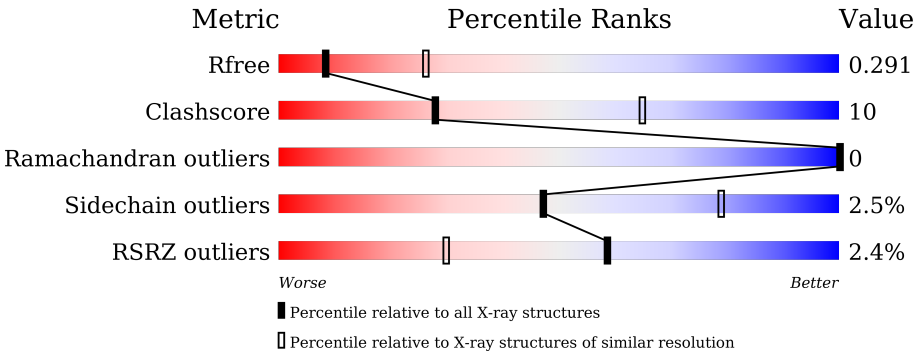
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	207	2% 71% 19% 10%
1	B	207	2% 70% 22% 8%
1	C	207	% 72% 21% • 5%
1	D	207	2% 68% 27% 5%
1	E	207	3% 68% 27% 5%
1	F	207	3% 67% 19% • 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9186 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 LysR family transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1492	959	254	270	9			
1	B	190	Total	C	N	O	S	0	1	0
			1526	981	257	278	10			
1	C	196	Total	C	N	O	S	0	0	0
			1565	1000	267	289	9			
1	D	197	Total	C	N	O	S	0	0	0
			1575	1008	270	288	9			
1	E	197	Total	C	N	O	S	0	0	0
			1573	1006	268	290	9			
1	F	181	Total	C	N	O	S	0	1	0
			1455	936	249	261	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	GLY	-	expression tag	UNP A0A087IWB4
A	86	ALA	-	expression tag	UNP A0A087IWB4
A	87	MET	-	expression tag	UNP A0A087IWB4
A	227	SER	CYS	engineered mutation	UNP A0A087IWB4
B	85	GLY	-	expression tag	UNP A0A087IWB4
B	86	ALA	-	expression tag	UNP A0A087IWB4
B	87	MET	-	expression tag	UNP A0A087IWB4
B	227	SER	CYS	engineered mutation	UNP A0A087IWB4
C	85	GLY	-	expression tag	UNP A0A087IWB4
C	86	ALA	-	expression tag	UNP A0A087IWB4
C	87	MET	-	expression tag	UNP A0A087IWB4
C	227	SER	CYS	engineered mutation	UNP A0A087IWB4
D	85	GLY	-	expression tag	UNP A0A087IWB4
D	86	ALA	-	expression tag	UNP A0A087IWB4
D	87	MET	-	expression tag	UNP A0A087IWB4
D	227	SER	CYS	engineered mutation	UNP A0A087IWB4
E	85	GLY	-	expression tag	UNP A0A087IWB4

Continued on next page...

Continued from previous page...

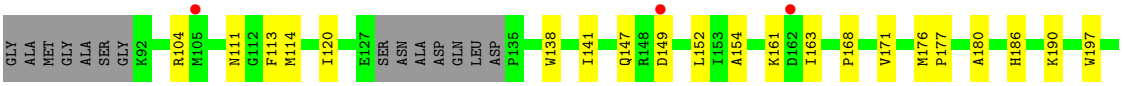
Chain	Residue	Modelled	Actual	Comment	Reference
E	86	ALA	-	expression tag	UNP A0A087IWB4
E	87	MET	-	expression tag	UNP A0A087IWB4
E	227	SER	CYS	engineered mutation	UNP A0A087IWB4
F	85	GLY	-	expression tag	UNP A0A087IWB4
F	86	ALA	-	expression tag	UNP A0A087IWB4
F	87	MET	-	expression tag	UNP A0A087IWB4
F	227	SER	CYS	engineered mutation	UNP A0A087IWB4

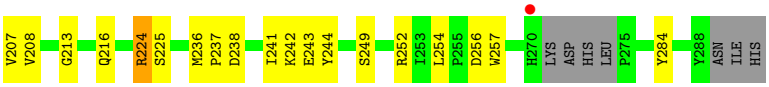
3 Residue-property plots (i)

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: LysR family transcriptional regulator

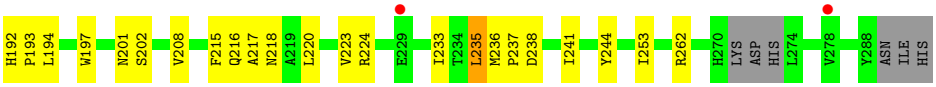
Chain A:





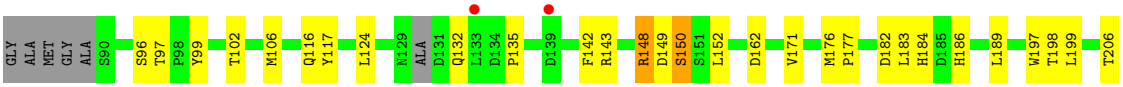
• Molecule 1: LysR family transcriptional regulator

Chain B:



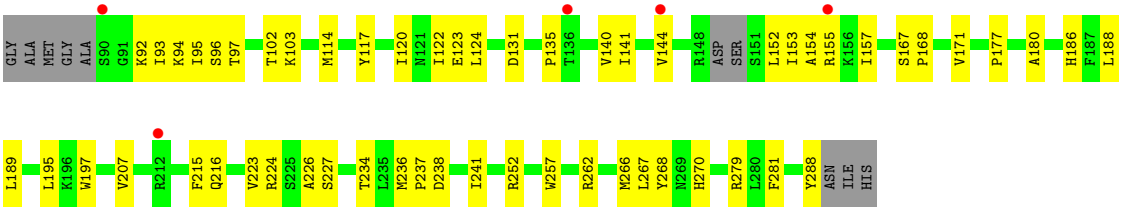
• Molecule 1: LysR family transcriptional regulator

Chain C:

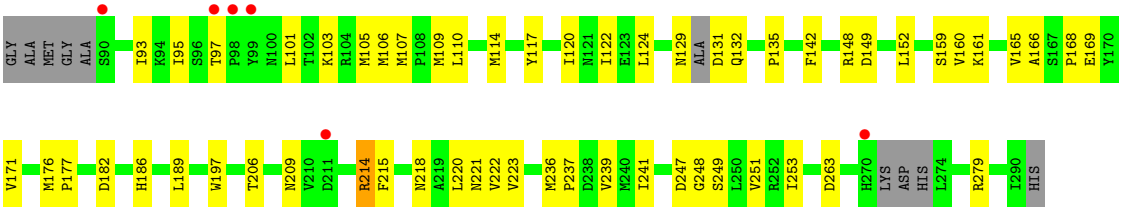


• Molecule 1: LysR family transcriptional regulator

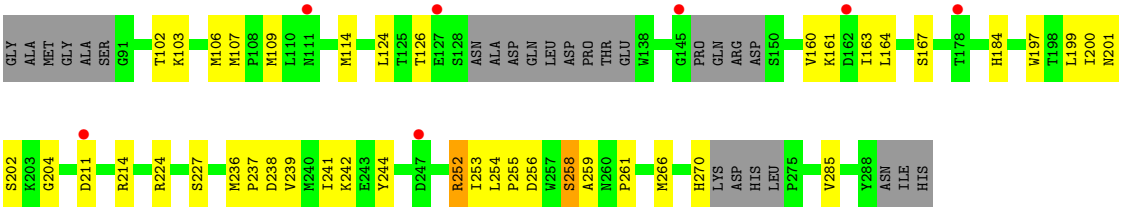
Chain D:



• Molecule 1: LysR family transcriptional regulator



• Molecule 1: LysR family transcriptional regulator



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	230.28Å 72.39Å 112.21Å 90.00° 118.71° 90.00°	Depositor
Resolution (Å)	38.93 – 2.99 38.93 – 2.99	Depositor EDS
% Data completeness (in resolution range)	87.7 (38.93-2.99) 86.1 (38.93-2.99)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.237 , 0.291 0.237 , 0.291	Depositor DCC
R_{free} test set	1478 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	47.5	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , -15.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.059 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	9186	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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	0.26	0/1527	0.46	0/2070
1	B	0.24	0/1560	0.43	0/2116
1	C	0.25	0/1600	0.44	0/2170
1	D	0.24	0/1612	0.45	0/2188
1	E	0.24	0/1608	0.44	0/2182
1	F	0.25	0/1487	0.45	0/2012
All	All	0.25	0/9394	0.44	0/12738

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	1492	0	1508	26	1
1	B	1526	0	1538	34	0
1	C	1565	0	1570	28	0
1	D	1575	0	1584	33	0
1	E	1573	0	1580	45	0
1	F	1455	0	1474	36	0
All	All	9186	0	9254	183	1

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 10.

All (183) 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:F:252:ARG:NH2	1:F:255:PRO:O	2.13	0.82
1:A:104:ARG:HH21	1:A:243:GLU:HG2	1.45	0.82
1:E:117:TYR:O	1:F:214[B]:ARG:NH2	2.16	0.79
1:E:189:LEU:HD12	1:E:215:PHE:HB3	1.71	0.72
1:A:244:TYR:HB3	1:A:249:SER:HB3	1.73	0.69
1:C:135:PRO:HB3	1:C:152:LEU:HD11	1.74	0.69
1:D:135:PRO:HB3	1:D:152:LEU:HD21	1.75	0.69
1:E:114:MET:O	1:F:214[A]:ARG:NH2	2.25	0.69
1:C:177:PRO:HB3	1:C:182:ASP:HB2	1.76	0.68
1:E:105:MET:HE3	1:E:239:VAL:HG11	1.76	0.67
1:E:171:VAL:HG22	1:E:176:MET:HE1	1.77	0.67
1:E:101:LEU:HB3	1:E:105:MET:HG3	1.77	0.66
1:E:120:ILE:O	1:F:214[B]:ARG:NH1	2.28	0.66
1:F:253:ILE:HG22	1:F:254:LEU:HG	1.78	0.66
1:C:279:ARG:NH1	1:C:283:ASP:OD1	2.32	0.63
1:A:147:GLN:NE2	1:A:152:LEU:O	2.32	0.62
1:E:105:MET:HE1	1:E:239:VAL:HG21	1.82	0.62
1:D:224:ARG:HD3	1:D:241:ILE:HG22	1.82	0.61
1:C:197:TRP:HB3	1:C:199:LEU:HD11	1.83	0.61
1:C:198:THR:HG22	1:C:208:VAL:HG22	1.82	0.60
1:A:254:LEU:HB3	1:A:257:TRP:HD1	1.68	0.58
1:B:165:VAL:HG11	1:B:241:ILE:HD12	1.84	0.58
1:F:236:MET:HB3	1:F:241:ILE:HD13	1.84	0.58
1:F:197:TRP:HB3	1:F:199:LEU:HD11	1.86	0.58
1:B:103:LYS:HE3	1:B:104:ARG:HH21	1.70	0.57
1:C:184:HIS:ND1	1:C:211:ASP:OD2	2.37	0.57
1:D:157:ILE:HD11	1:D:266:MET:HB2	1.86	0.56
1:C:171:VAL:HG23	1:C:176:MET:HG3	1.86	0.56
1:F:201:ASN:OD1	1:F:204:GLY:N	2.37	0.56
1:B:220:LEU:HA	1:B:223:VAL:HG22	1.87	0.56
1:D:92:LYS:HE2	1:D:94:LYS:HE2	1.87	0.56
1:A:236:MET:HG3	1:A:237:PRO:HD2	1.88	0.55
1:E:177:PRO:HB3	1:E:182:ASP:HB2	1.88	0.55
1:F:164:LEU:O	1:F:252:ARG:HG3	2.05	0.55
1:F:258:SER:OG	1:F:259:ALA:N	2.40	0.55
1:F:236:MET:HG2	1:F:241:ILE:HG23	1.88	0.55
1:E:168:PRO:HG3	1:E:251:VAL:HG13	1.89	0.54
1:F:163:ILE:HB	1:F:252:ARG:HD2	1.89	0.54
1:C:189:LEU:HD22	1:C:215:PHE:HB3	1.88	0.54
1:B:107[B]:MET:HE2	1:C:222:VAL:HG12	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:ILE:HG23	1:D:120:ILE:HD11	1.89	0.54
1:E:165:VAL:HG11	1:E:241:ILE:HD12	1.89	0.54
1:C:152:LEU:HD13	1:C:267:LEU:HD23	1.90	0.54
1:C:162:ASP:OD2	1:C:262:ARG:NH1	2.41	0.54
1:E:218:ASN:HD21	1:F:126:THR:H	1.54	0.53
1:A:180:ALA:HB3	1:A:207:VAL:HG21	1.91	0.53
1:A:254:LEU:HB3	1:A:257:TRP:CD1	2.43	0.53
1:E:149:ASP:OD2	1:E:149:ASP:N	2.34	0.53
1:A:243:GLU:H	1:A:243:GLU:CD	2.12	0.52
1:B:194:LEU:HD13	1:B:235:LEU:HD23	1.92	0.52
1:B:95:ILE:HD11	1:B:110:LEU:HD21	1.91	0.52
1:D:180:ALA:HB3	1:D:207:VAL:HG21	1.91	0.52
1:B:160:VAL:HG21	1:B:237:PRO:HB3	1.92	0.52
1:E:171:VAL:HG21	1:E:251:VAL:HG21	1.92	0.52
1:B:123:GLU:OE2	1:C:216:GLN:NE2	2.42	0.51
1:E:95:ILE:HD11	1:E:110:LEU:HD21	1.92	0.51
1:B:190:LYS:HB2	1:B:216:GLN:HG2	1.91	0.51
1:D:238:ASP:OD2	1:D:238:ASP:N	2.43	0.51
1:C:116:GLN:HB2	1:C:117:TYR:CD2	2.46	0.51
1:E:97:THR:HG22	1:E:142:PHE:CD2	2.46	0.51
1:F:109:MET:SD	1:F:285:VAL:HG22	2.50	0.51
1:E:131:ASP:HA	1:E:148:ARG:NH2	2.26	0.51
1:B:223:VAL:HG23	1:B:236:MET:HE1	1.92	0.51
1:B:236:MET:HB3	1:B:241:ILE:HD13	1.92	0.51
1:E:176:MET:HB3	1:E:177:PRO:HD2	1.93	0.50
1:A:224:ARG:HB2	1:A:236:MET:SD	2.51	0.50
1:D:144:VAL:HG11	1:D:262:ARG:HE	1.76	0.50
1:B:233:ILE:HD12	1:B:253:ILE:HD13	1.93	0.49
1:E:160:VAL:HG21	1:E:237:PRO:HB3	1.94	0.49
1:D:97:THR:HG21	1:D:102:THR:HG23	1.95	0.49
1:B:135:PRO:HB3	1:B:152:LEU:HD11	1.94	0.49
1:B:197:TRP:O	1:B:208:VAL:HA	2.13	0.48
1:C:143:ARG:HD2	1:C:148:ARG:NH1	2.28	0.48
1:C:243:GLU:OE1	1:C:243:GLU:N	2.38	0.48
1:A:177:PRO:HD3	1:A:186:HIS:CE1	2.49	0.48
1:C:236:MET:HG3	1:C:237:PRO:HD2	1.96	0.48
1:D:188:LEU:HD22	1:D:197:TRP:CZ3	2.49	0.48
1:E:149:ASP:OD2	1:E:152:LEU:HD12	2.14	0.48
1:D:95:ILE:HB	1:D:124:LEU:HD12	1.95	0.48
1:F:163:ILE:HB	1:F:252:ARG:HH11	1.79	0.48
1:B:123:GLU:HG3	1:C:216:GLN:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PRO:O	1:A:241:ILE:HG12	2.14	0.47
1:C:183:LEU:HD12	1:C:209:ASN:HD22	1.79	0.47
1:C:266:MET:SD	1:C:285:VAL:HG21	2.54	0.47
1:E:103:LYS:HA	1:E:107:MET:HG2	1.96	0.47
1:E:197:TRP:HB2	1:E:209:ASN:HB3	1.95	0.47
1:A:111:ASN:ND2	1:D:226:ALA:HA	2.30	0.47
1:B:103:LYS:HA	1:B:107[B]:MET:SD	2.55	0.47
1:E:114:MET:O	1:F:214[B]:ARG:NH2	2.48	0.47
1:F:184:HIS:ND1	1:F:211:ASP:OD2	2.36	0.47
1:C:224:ARG:HB2	1:C:236:MET:SD	2.54	0.47
1:D:96:SER:HB3	1:D:141:ILE:HG23	1.95	0.47
1:D:167:SER:HB3	1:D:227:SER:O	2.15	0.46
1:F:239:VAL:HA	1:F:242:LYS:HE3	1.97	0.46
1:E:93:ILE:HB	1:E:122:ILE:HD13	1.97	0.46
1:E:97:THR:HG22	1:E:142:PHE:HD2	1.81	0.46
1:B:95:ILE:HG22	1:B:140:VAL:HB	1.97	0.46
1:D:93:ILE:HD11	1:D:122:ILE:HG13	1.98	0.46
1:E:214:ARG:NH1	1:F:114:MET:O	2.49	0.46
1:B:177:PRO:HB3	1:B:182:ASP:HB2	1.98	0.46
1:B:236:MET:HG3	1:B:237:PRO:HD2	1.97	0.46
1:A:138:TRP:HB2	1:A:141:ILE:HD11	1.97	0.46
1:B:107[B]:MET:HB2	1:B:108:PRO:HD3	1.98	0.46
1:E:166:ALA:HB3	1:E:253:ILE:HD11	1.97	0.46
1:C:102:THR:HA	1:C:106:MET:HG2	1.98	0.45
1:D:153:ILE:O	1:D:267:LEU:HA	2.16	0.45
1:B:189:LEU:N	1:B:233:ILE:O	2.41	0.45
1:D:177:PRO:HD3	1:D:186:HIS:NE2	2.31	0.45
1:D:93:ILE:HD12	1:D:95:ILE:HG13	1.97	0.45
1:D:154:ALA:C	1:D:155:ARG:HD2	2.37	0.45
1:D:114:MET:HG2	1:D:122:ILE:HD13	1.99	0.45
1:D:195:LEU:HD11	1:D:216:GLN:HG3	1.98	0.45
1:E:129:ASN:HB3	1:E:132:GLN:CD	2.37	0.45
1:F:103:LYS:HB2	1:F:103:LYS:HE2	1.73	0.44
1:F:202:SER:N	1:F:256:ASP:OD2	2.50	0.44
1:F:163:ILE:CG2	1:F:252:ARG:HH11	2.30	0.44
1:A:154:ALA:HB3	1:C:206:THR:OG1	2.18	0.44
1:B:236:MET:HE3	1:B:236:MET:HB2	1.95	0.44
1:B:224:ARG:HD2	1:B:244:TYR:CE2	2.52	0.44
1:D:140:VAL:HG21	1:D:281:PHE:CE1	2.52	0.44
1:D:189:LEU:HB2	1:D:234:THR:OG1	2.17	0.44
1:A:111:ASN:HD21	1:D:226:ALA:HA	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:MET:HG2	1:E:186:HIS:CE1	2.53	0.44
1:D:215:PHE:CD2	1:D:223:VAL:HG12	2.53	0.44
1:F:160:VAL:CG1	1:F:237:PRO:HB3	2.48	0.44
1:F:238:ASP:OD1	1:F:238:ASP:N	2.49	0.44
1:F:266:MET:CE	1:F:285:VAL:HG11	2.48	0.44
1:B:154:ALA:HB3	1:E:206:THR:HB	2.00	0.43
1:C:149:ASP:OD2	1:C:150:SER:N	2.51	0.43
1:C:177:PRO:HG3	1:C:186:HIS:CD2	2.54	0.43
1:D:168:PRO:HA	1:D:171:VAL:HG22	1.99	0.43
1:D:279:ARG:HH11	1:D:279:ARG:HB3	1.83	0.43
1:E:105:MET:CE	1:E:239:VAL:HG21	2.47	0.43
1:E:135:PRO:HG3	1:E:152:LEU:HD11	2.01	0.43
1:B:189:LEU:HD22	1:B:215:PHE:HB3	2.00	0.43
1:A:147:GLN:OE1	1:C:206:THR:OG1	2.37	0.43
1:E:159:SER:HB3	1:E:263:ASP:HA	2.01	0.43
1:E:221:ASN:HB2	1:F:103:LYS:HD2	2.00	0.43
1:A:176:MET:HG2	1:A:177:PRO:HD2	2.00	0.43
1:C:212:ARG:CZ	1:C:212:ARG:HB2	2.48	0.43
1:E:222:VAL:HG21	1:F:124:LEU:HD23	2.01	0.43
1:F:200:ILE:HG13	1:F:201:ASN:N	2.34	0.43
1:E:129:ASN:OD1	1:E:132:GLN:N	2.52	0.43
1:F:102:THR:HA	1:F:106:MET:HG2	2.01	0.42
1:F:224:ARG:HD2	1:F:244:TYR:CE1	2.54	0.42
1:A:163:ILE:HB	1:A:252:ARG:HE	1.84	0.42
1:D:236:MET:HG3	1:D:237:PRO:HD2	2.02	0.42
1:E:247:ASP:CG	1:E:248:GLY:H	2.22	0.42
1:A:168:PRO:HA	1:A:171:VAL:HG22	2.00	0.42
1:B:217:ALA:HA	1:C:124:LEU:O	2.18	0.42
1:B:162:ASP:OD1	1:B:262:ARG:NH1	2.52	0.42
1:E:106:MET:O	1:E:109:MET:HB3	2.20	0.42
1:E:236:MET:HB3	1:E:241:ILE:HD13	2.02	0.42
1:A:113:PHE:HE2	1:A:120:ILE:HG21	1.84	0.42
1:E:161:LYS:HE2	1:E:161:LYS:HB3	1.88	0.42
1:A:225:SER:HB2	1:D:103:LYS:HE2	2.02	0.42
1:B:192:HIS:HB3	1:B:218:ASN:HA	2.01	0.42
1:B:102:THR:O	1:B:107[B]:MET:HG3	2.20	0.41
1:B:164:LEU:HG	1:B:235:LEU:HD12	2.00	0.41
1:A:197:TRP:O	1:A:208:VAL:HA	2.19	0.41
1:E:247:ASP:OD2	1:E:249:SER:HB2	2.19	0.41
1:F:161:LYS:HG3	1:F:261:PRO:HG3	2.02	0.41
1:F:163:ILE:CG2	1:F:252:ARG:NH1	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASP:O	1:A:242:LYS:HG3	2.20	0.41
1:B:143:ARG:NH1	1:B:146:PRO:O	2.53	0.41
1:D:153:ILE:HG21	1:D:268:TYR:CZ	2.56	0.41
1:D:236:MET:HB2	1:D:236:MET:HE2	1.93	0.41
1:E:97:THR:CG2	1:E:106:MET:HE1	2.51	0.41
1:E:220:LEU:HA	1:E:223:VAL:HG22	2.02	0.41
1:B:201:ASN:OD1	1:B:202:SER:N	2.54	0.41
1:B:238:ASP:OD1	1:B:238:ASP:N	2.54	0.41
1:E:159:SER:CB	1:E:263:ASP:HA	2.50	0.41
1:A:213:GLY:H	1:A:216:GLN:HE21	1.69	0.41
1:C:97:THR:HG22	1:C:142:PHE:HB2	2.03	0.40
1:F:238:ASP:O	1:F:242:LYS:HB3	2.21	0.40
1:E:218:ASN:ND2	1:F:126:THR:H	2.19	0.40
1:F:102:THR:O	1:F:107:MET:HG2	2.22	0.40
1:A:104:ARG:HH21	1:A:243:GLU:CG	2.24	0.40
1:D:117:TYR:O	1:D:120:ILE:HG22	2.21	0.40
1:F:167:SER:HB2	1:F:227:SER:O	2.21	0.40
1:A:190:LYS:O	1:A:216:GLN:HA	2.22	0.40
1:B:192:HIS:CE1	1:B:193:PRO:HB3	2.57	0.40
1:D:95:ILE:HD13	1:D:95:ILE:HG21	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ASP:OD1	1:A:284:TYR:OH[4_444]	2.05	0.15

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	180/207 (87%)	171 (95%)	9 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	183/207 (88%)	179 (98%)	4 (2%)	0	100	100
1	C	190/207 (92%)	180 (95%)	10 (5%)	0	100	100
1	D	193/207 (93%)	186 (96%)	7 (4%)	0	100	100
1	E	191/207 (92%)	177 (93%)	14 (7%)	0	100	100
1	F	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
All	All	1111/1242 (90%)	1060 (95%)	51 (5%)	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	167/182 (92%)	163 (98%)	4 (2%)	49	79
1	B	171/182 (94%)	169 (99%)	2 (1%)	71	90
1	C	176/182 (97%)	169 (96%)	7 (4%)	31	68
1	D	176/182 (97%)	170 (97%)	6 (3%)	37	72
1	E	177/182 (97%)	173 (98%)	4 (2%)	50	80
1	F	162/182 (89%)	159 (98%)	3 (2%)	57	84
All	All	1029/1092 (94%)	1003 (98%)	26 (2%)	47	79

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	MET
1	A	149	ASP
1	A	161	LYS
1	A	224	ARG
1	B	150	SER
1	B	235	LEU
1	C	96	SER
1	C	99	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	132	GLN
1	C	148	ARG
1	C	150	SER
1	C	212	ARG
1	C	249	SER
1	D	123	GLU
1	D	131	ASP
1	D	252	ARG
1	D	257	TRP
1	D	270	HIS
1	D	288	TYR
1	E	124	LEU
1	E	169	GLU
1	E	214	ARG
1	E	279	ARG
1	F	252	ARG
1	F	258	SER
1	F	270	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	HIS
1	B	172	ASN
1	E	121	ASN

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

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	186/207 (89%)	0.20	4 (2%)	62	33	23, 43, 83, 95	0
1	B	190/207 (91%)	0.13	4 (2%)	63	34	18, 39, 67, 89	0
1	C	196/207 (94%)	0.18	2 (1%)	82	59	14, 44, 80, 101	0
1	D	197/207 (95%)	0.30	5 (2%)	57	29	28, 58, 94, 101	0
1	E	197/207 (95%)	0.25	6 (3%)	50	22	22, 46, 80, 104	0
1	F	181/207 (87%)	0.32	7 (3%)	39	15	26, 55, 81, 116	0
All	All	1147/1242 (92%)	0.23	28 (2%)	59	30	14, 48, 83, 116	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	90	SER	11.4
1	E	90	SER	9.0
1	C	133	LEU	3.9
1	F	178	THR	3.8
1	F	247	ASP	3.7
1	E	99	TYR	3.6
1	F	111	ASN	3.5
1	B	278	VAL	3.0
1	A	162	ASP	2.9
1	B	181	GLU	2.8
1	A	149	ASP	2.8
1	A	270	HIS	2.7
1	A	105	MET	2.6
1	C	139	ASP	2.6
1	E	97	THR	2.5
1	F	162	ASP	2.4
1	F	211	ASP	2.4
1	F	127	GLU	2.4
1	E	211	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	270	HIS	2.2
1	D	136	THR	2.2
1	E	98	PRO	2.2
1	B	229	GLU	2.2
1	D	212	ARG	2.1
1	F	145	GLY	2.1
1	D	155	ARG	2.1
1	B	145	GLY	2.1
1	D	144	VAL	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.