Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:00 pm BST

PDB ID	:	3D8U
Title	:	The crystal structure of a PurR family transcriptional regulator from Vibrio parahaemolyticus RIMD 2210633
Authors	:	Tan, K.; Hatzos, C.; Moy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2008-05-23
Resolution	:	2.88 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 ①) were used in the production of this report:

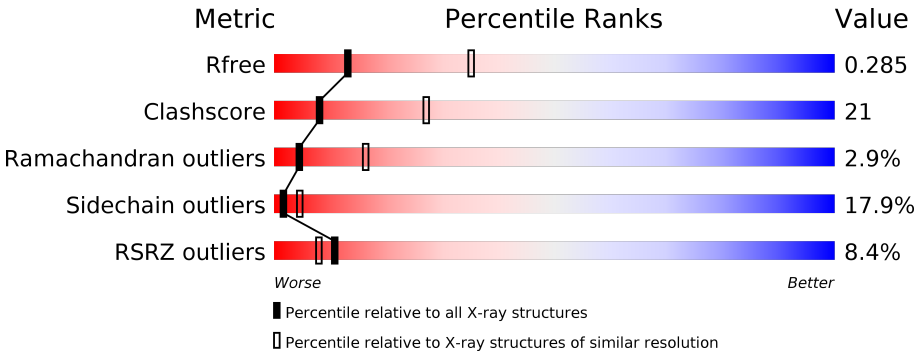
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.88 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 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	275	8%, 52%, 35%, 8%
1	B	275	8%, 63%, 27%, 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3935 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 PurR transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	Se	0	0	0
			1964	1238	342	375	5	4			
1	B	270	Total	C	N	O	S	Se	0	1	0
			1971	1241	345	375	5	5			

There are 6 discrepancies between the modelled and reference sequences:

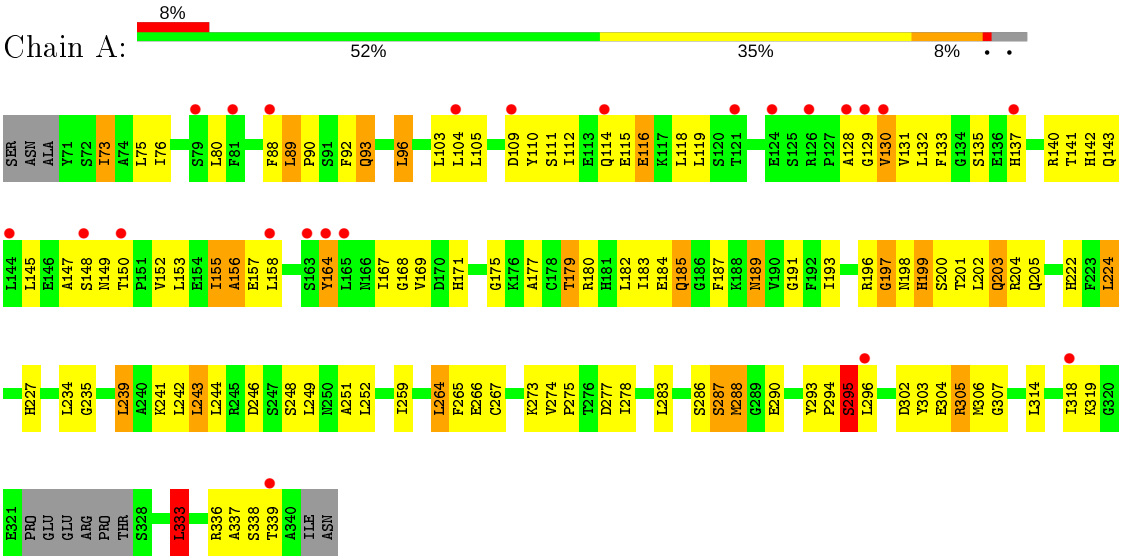
Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SER	-	EXPRESSION TAG	UNP Q87JL7
A	69	ASN	-	EXPRESSION TAG	UNP Q87JL7
A	70	ALA	-	EXPRESSION TAG	UNP Q87JL7
B	68	SER	-	EXPRESSION TAG	UNP Q87JL7
B	69	ASN	-	EXPRESSION TAG	UNP Q87JL7
B	70	ALA	-	EXPRESSION TAG	UNP Q87JL7

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 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.

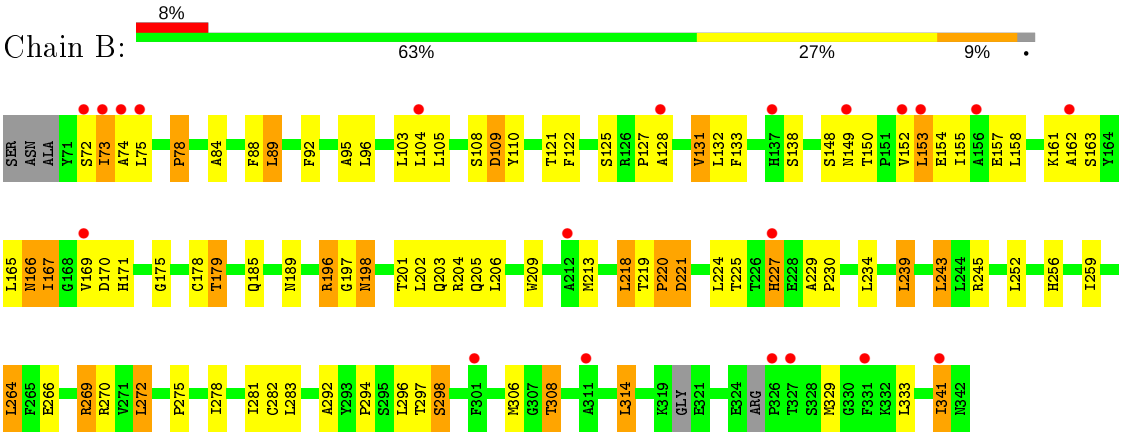
- Molecule 1: PurR transcriptional regulator

Chain A:



- Molecule 1: PurR transcriptional regulator

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.26Å 126.26Å 83.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.30 – 2.88 41.33 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.5 (41.30-2.88) 98.5 (41.33-2.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.283 0.212 , 0.285	Depositor DCC
R_{free} test set	891 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	79.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 110.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3935	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% 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	0.65	0/1998	0.77	1/2700 (0.0%)
1	B	0.67	0/2007	0.82	3/2714 (0.1%)
All	All	0.66	0/4005	0.80	4/5414 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	333	LEU	CA-CB-CG	5.29	127.46	115.30
1	B	269	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	245	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	272	LEU	CA-CB-CG	5.13	127.09	115.30

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	1964	0	1878	93	0
1	B	1971	0	1838	72	0
All	All	3935	0	3716	163	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 21.

All (163) 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:A:185:GLN:HA	1:A:185:GLN:NE2	1.64	1.10
1:A:185:GLN:HA	1:A:185:GLN:HE21	0.84	1.01
1:A:185:GLN:CA	1:A:185:GLN:HE21	1.77	0.98
1:B:196:ARG:HH12	1:B:201:THR:HB	1.27	0.97
1:A:131:VAL:HG12	1:A:153:LEU:HB3	1.45	0.96
1:B:256:HIS:HB2	1:B:259:ILE:HD12	1.58	0.85
1:A:152:VAL:O	1:A:164:TYR:HB2	1.76	0.84
1:A:143:GLN:O	1:A:147:ALA:HB2	1.83	0.79
1:B:157:GLU:HG2	1:B:169:VAL:O	1.82	0.79
1:A:333:LEU:HD13	1:A:333:LEU:O	1.85	0.77
1:A:197:GLY:O	1:A:198:ASN:HB2	1.85	0.76
1:B:175:GLY:O	1:B:179:THR:HG22	1.88	0.74
1:A:131:VAL:HG13	1:A:314:LEU:HD11	1.70	0.73
1:B:179:THR:HG21	1:B:209:TRP:HA	1.70	0.73
1:B:227:HIS:CD2	1:B:227:HIS:H	2.06	0.72
1:B:95:ALA:HB2	1:B:308:THR:HG22	1.72	0.72
1:A:296:LEU:O	1:A:336:ARG:HD2	1.90	0.71
1:B:281:ILE:HG13	1:B:297:THR:HG22	1.71	0.71
1:A:239:LEU:HD22	1:A:243:LEU:HD22	1.74	0.69
1:A:294:PRO:O	1:A:295:SER:O	2.11	0.68
1:B:266:GLU:O	1:B:270:ARG:HG3	1.92	0.68
1:A:275:PRO:HA	1:A:278:ILE:O	1.95	0.67
1:B:202:LEU:HD21	1:B:225:THR:HG21	1.75	0.67
1:A:155:ILE:HA	1:A:167:ILE:O	1.95	0.67
1:A:202:LEU:HA	1:A:205:GLN:HE21	1.60	0.66
1:B:108:SER:O	1:B:110:TYR:N	2.30	0.65
1:A:189:ASN:HD22	1:A:189:ASN:C	2.00	0.63
1:B:153:LEU:HD23	1:B:166:ASN:HA	1.81	0.62
1:B:178:CYS:HB3	1:B:281:ILE:HD13	1.82	0.62
1:B:72:SER:O	1:B:128:ALA:HB3	1.99	0.62
1:B:202:LEU:HD21	1:B:225:THR:CG2	2.30	0.62
1:B:275:PRO:HA	1:B:278:ILE:O	2.01	0.61
1:A:224:LEU:HD22	1:A:242:LEU:CD2	2.31	0.61
1:A:175:GLY:O	1:A:179:THR:HG23	2.01	0.60
1:A:131:VAL:CG1	1:A:153:LEU:HB3	2.27	0.60
1:B:227:HIS:HD2	1:B:227:HIS:H	1.46	0.60
1:A:177:ALA:HA	1:A:180:ARG:NH2	2.17	0.60
1:A:180:ARG:O	1:A:184:GLU:HG2	2.01	0.60
1:B:198:ASN:HD22	1:B:198:ASN:N	2.00	0.60
1:B:239:LEU:HD22	1:B:243:LEU:HD22	1.82	0.60
1:A:304:GLU:H	1:A:304:GLU:CD	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ASP:N	1:B:221:ASP:OD1	2.36	0.58
1:B:132:LEU:O	1:B:154:GLU:HA	2.03	0.58
1:A:147:ALA:C	1:A:149:ASN:H	2.07	0.58
1:A:183:ILE:C	1:A:185:GLN:H	2.07	0.58
1:B:197:GLY:HA3	1:B:202:LEU:CD2	2.34	0.57
1:A:274:VAL:O	1:A:294:PRO:HG2	2.04	0.57
1:A:290:GLU:HG2	1:A:336:ARG:NH2	2.19	0.57
1:A:75:LEU:HD11	1:A:133:PHE:HE2	1.70	0.57
1:A:294:PRO:C	1:A:295:SER:O	2.43	0.56
1:A:185:GLN:HB3	1:A:187:PHE:HD1	1.71	0.56
1:A:293:TYR:CE2	1:B:269:ARG:HG3	2.40	0.56
1:A:314:LEU:O	1:A:318:ILE:HG23	2.05	0.56
1:A:93:GLN:HB3	1:A:103:LEU:HD22	1.88	0.56
1:B:213:MSE:HE3	1:B:218:LEU:HB3	1.86	0.56
1:B:73:ILE:HD12	1:B:96:LEU:HD21	1.88	0.56
1:A:224:LEU:HD22	1:A:242:LEU:HD21	1.88	0.56
1:A:156:ALA:O	1:A:168:GLY:HA3	2.06	0.56
1:B:201:THR:O	1:B:205:GLN:HG3	2.06	0.55
1:A:143:GLN:O	1:A:147:ALA:CB	2.54	0.55
1:B:155:ILE:CG2	1:B:306:MSE:HE3	2.38	0.54
1:B:155:ILE:HG21	1:B:306:MSE:HE3	1.88	0.53
1:B:306:MSE:HB2	1:B:329[B]:MSE:HE1	1.90	0.53
1:B:185:GLN:HE22	1:B:341:ILE:HG22	1.73	0.53
1:A:287:SER:HA	1:A:290:GLU:HG3	1.91	0.52
1:B:197:GLY:CA	1:B:202:LEU:CD2	2.88	0.52
1:B:202:LEU:HA	1:B:205:GLN:HE21	1.75	0.51
1:B:84:ALA:O	1:B:88:PHE:CB	2.60	0.50
1:B:270:ARG:HB2	1:B:272:LEU:CD2	2.41	0.50
1:A:112:ILE:O	1:A:116:GLU:OE2	2.30	0.50
1:B:197:GLY:HA3	1:B:202:LEU:HD22	1.94	0.49
1:A:175:GLY:O	1:A:179:THR:CG2	2.61	0.49
1:A:147:ALA:C	1:A:149:ASN:N	2.66	0.48
1:A:75:LEU:HD13	1:A:131:VAL:HG23	1.95	0.48
1:B:197:GLY:HA2	1:B:202:LEU:HB3	1.96	0.48
1:B:270:ARG:HB2	1:B:272:LEU:HD23	1.96	0.48
1:A:109:ASP:O	1:A:110:TYR:HB2	2.14	0.48
1:A:111:SER:HB3	1:A:114:GLN:CB	2.44	0.48
1:B:84:ALA:O	1:B:88:PHE:HB2	2.13	0.48
1:A:302:ASP:OD1	1:A:304:GLU:HG2	2.14	0.47
1:A:73:ILE:HD13	1:A:73:ILE:O	2.14	0.47
1:B:197:GLY:CA	1:B:202:LEU:HD23	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:HIS:H	1:A:227:HIS:CD2	2.30	0.47
1:B:227:HIS:N	1:B:227:HIS:CD2	2.79	0.47
1:B:230:PRO:HG3	1:B:256:HIS:CD2	2.49	0.47
1:A:75:LEU:CD1	1:A:131:VAL:HG23	2.45	0.46
1:A:115:GLU:O	1:A:119:LEU:HB2	2.15	0.46
1:A:116:GLU:HG3	1:A:141:THR:CB	2.46	0.46
1:B:148:SER:C	1:B:150:THR:H	2.19	0.46
1:B:95:ALA:HB2	1:B:308:THR:CG2	2.42	0.46
1:B:78:PRO:HB2	1:B:110:TYR:CE2	2.51	0.46
1:B:109:ASP:O	1:B:110:TYR:C	2.54	0.46
1:B:197:GLY:CA	1:B:202:LEU:HD22	2.46	0.46
1:A:130:VAL:HG13	1:A:152:VAL:HG13	1.98	0.46
1:A:111:SER:HB3	1:A:114:GLN:HB2	1.97	0.46
1:A:274:VAL:HB	1:A:278:ILE:O	2.16	0.46
1:A:88:PHE:CD1	1:A:306:MSE:HE3	2.51	0.46
1:B:122:PHE:O	1:B:125:SER:HB3	2.15	0.46
1:B:198:ASN:CG	1:B:227:HIS:HB3	2.36	0.45
1:A:145:LEU:C	1:A:147:ALA:H	2.19	0.45
1:A:185:GLN:HB3	1:A:187:PHE:CD1	2.51	0.45
1:B:108:SER:OG	1:B:108:SER:O	2.34	0.45
1:A:88:PHE:CD1	1:A:307:GLY:HA2	2.51	0.45
1:A:88:PHE:HA	1:A:303:TYR:O	2.16	0.45
1:A:337:ALA:O	1:A:339:THR:N	2.49	0.45
1:B:264:LEU:HD21	1:B:294:PRO:HD2	1.99	0.45
1:A:305:ARG:CG	1:A:305:ARG:HH11	2.30	0.45
1:B:153:LEU:HA	1:B:165:LEU:O	2.17	0.45
1:A:290:GLU:HG2	1:A:336:ARG:CZ	2.47	0.44
1:B:73:ILE:C	1:B:73:ILE:HD13	2.37	0.44
1:B:75:LEU:HD21	1:B:89:LEU:HD21	1.99	0.44
1:A:294:PRO:O	1:A:295:SER:C	2.56	0.44
1:A:333:LEU:CD1	1:A:333:LEU:O	2.62	0.44
1:A:264:LEU:O	1:A:267:CYS:HB2	2.16	0.44
1:A:191:GLY:HA2	1:A:222:HIS:O	2.16	0.44
1:A:193:ILE:HG13	1:A:252:LEU:HD11	1.98	0.44
1:B:167:ILE:HD12	1:B:306:MSE:HG3	2.00	0.44
1:A:273:LYS:O	1:A:277:ASP:HB2	2.18	0.44
1:B:197:GLY:C	1:B:198:ASN:HD22	2.21	0.44
1:B:105:LEU:O	1:B:122:PHE:HZ	2.01	0.43
1:B:219:THR:HG22	1:B:221:ASP:OD1	2.17	0.43
1:A:183:ILE:C	1:A:185:GLN:N	2.71	0.43
1:A:202:LEU:O	1:A:202:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLY:HA3	1:B:202:LEU:HD23	1.99	0.43
1:A:189:ASN:ND2	1:A:249:LEU:HD12	2.33	0.43
1:A:304:GLU:N	1:A:304:GLU:CD	2.71	0.43
1:B:170:ASP:C	1:B:170:ASP:OD2	2.57	0.43
1:B:171:HIS:CD2	1:B:201:THR:HG23	2.53	0.43
1:A:196:ARG:HA	1:A:196:ARG:HD3	1.82	0.43
1:A:288:MSE:HB3	1:A:288:MSE:HE3	1.66	0.43
1:A:286:SER:O	1:A:288:MSE:N	2.52	0.42
1:A:337:ALA:C	1:A:339:THR:H	2.22	0.42
1:B:75:LEU:HB2	1:B:131:VAL:HG13	2.01	0.42
1:B:282:CYS:HB3	1:B:298:SER:HB2	2.01	0.42
1:B:75:LEU:HD11	1:B:133:PHE:HE2	1.84	0.42
1:A:184:GLU:O	1:A:185:GLN:NE2	2.52	0.42
1:A:199:HIS:ND1	1:A:200:SER:N	2.68	0.42
1:A:89:LEU:O	1:A:92:PHE:HB3	2.20	0.41
1:A:177:ALA:HA	1:A:180:ARG:HH21	1.86	0.41
1:A:157:GLU:HG3	1:A:158:LEU:HG	2.02	0.41
1:A:197:GLY:C	1:A:199:HIS:H	2.24	0.41
1:A:235:GLY:HA2	1:A:259:ILE:HG23	2.02	0.41
1:B:74:ALA:HA	1:B:104:LEU:O	2.19	0.41
1:B:198:ASN:N	1:B:198:ASN:ND2	2.69	0.41
1:A:265:PHE:CD2	1:B:292:ALA:HA	2.54	0.41
1:A:128:ALA:HA	1:A:150:THR:HB	2.02	0.41
1:A:169:VAL:HG22	1:A:171:HIS:NE2	2.36	0.41
1:B:219:THR:HA	1:B:220:PRO:HD3	1.60	0.41
1:A:293:TYR:HA	1:A:294:PRO:C	2.40	0.41
1:A:137:HIS:HB2	1:A:142:HIS:CE1	2.55	0.41
1:A:246:ASP:OD1	1:A:248:SER:N	2.52	0.41
1:B:171:HIS:CG	1:B:201:THR:HG23	2.56	0.41
1:B:229:ALA:HB1	1:B:230:PRO:HD2	2.02	0.41
1:A:187:PHE:HB3	1:A:251:ALA:HB2	2.02	0.41
1:A:182:LEU:HD13	1:A:251:ALA:HB1	2.03	0.40
1:A:129:GLY:H	1:A:150:THR:HB	1.85	0.40
1:A:318:ILE:HG13	1:A:319:LYS:N	2.35	0.40
1:A:92:PHE:O	1:A:96:LEU:HB2	2.22	0.40
1:B:175:GLY:O	1:B:179:THR:CG2	2.63	0.40
1:B:314:LEU:HA	1:B:314:LEU:HD23	1.94	0.40
1:A:296:LEU:HA	1:A:296:LEU:HD12	1.83	0.40
1:A:200:SER:O	1:A:203:GLN:HG3	2.20	0.40
1:B:92:PHE:CZ	1:B:131:VAL:HG11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	260/275 (94%)	221 (85%)	31 (12%)	8 (3%)	4	15
1	B	265/275 (96%)	228 (86%)	30 (11%)	7 (3%)	5	19
All	All	525/550 (96%)	449 (86%)	61 (12%)	15 (3%)	4	16

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	SER
1	A	295	SER
1	A	338	SER
1	B	109	ASP
1	B	127	PRO
1	B	161	LYS
1	A	197	GLY
1	B	149	ASN
1	A	140	ARG
1	A	148	SER
1	A	156	ALA
1	B	162	ALA
1	B	78	PRO
1	B	220	PRO
1	A	90	PRO

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	200/225 (89%)	165 (82%)	35 (18%)	2 5
1	B	192/225 (85%)	157 (82%)	35 (18%)	1 4
All	All	392/450 (87%)	322 (82%)	70 (18%)	2 4

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ILE
1	A	76	ILE
1	A	80	LEU
1	A	89	LEU
1	A	93	GLN
1	A	96	LEU
1	A	104	LEU
1	A	105	LEU
1	A	116	GLU
1	A	118	LEU
1	A	130	VAL
1	A	132	LEU
1	A	135	SER
1	A	155	ILE
1	A	164	TYR
1	A	179	THR
1	A	185	GLN
1	A	189	ASN
1	A	199	HIS
1	A	201	THR
1	A	203	GLN
1	A	204	ARG
1	A	224	LEU
1	A	234	LEU
1	A	239	LEU
1	A	241	LYS
1	A	243	LEU
1	A	244	LEU
1	A	264	LEU
1	A	266	GLU
1	A	283	LEU
1	A	288	MSE
1	A	295	SER
1	A	305	ARG
1	A	333	LEU

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Mol	Chain	Res	Type
1	B	73	ILE
1	B	89	LEU
1	B	103	LEU
1	B	121	THR
1	B	131	VAL
1	B	138	SER
1	B	152	VAL
1	B	153	LEU
1	B	158	LEU
1	B	163	SER
1	B	166	ASN
1	B	167	ILE
1	B	179	THR
1	B	189	ASN
1	B	196	ARG
1	B	198	ASN
1	B	203	GLN
1	B	204	ARG
1	B	206	LEU
1	B	218	LEU
1	B	221	ASP
1	B	224	LEU
1	B	227	HIS
1	B	234	LEU
1	B	239	LEU
1	B	243	LEU
1	B	252	LEU
1	B	264	LEU
1	B	283	LEU
1	B	296	LEU
1	B	298	SER
1	B	308	THR
1	B	314	LEU
1	B	333	LEU
1	B	341	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	HIS
1	A	185	GLN
1	A	189	ASN

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Mol	Chain	Res	Type
1	A	205	GLN
1	A	216	ASN
1	A	222	HIS
1	A	227	HIS
1	A	268	HIS
1	B	198	ASN
1	B	205	GLN
1	B	227	HIS
1	B	268	HIS

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

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	260/275 (94%)	0.51	23 (8%)	10	7	73, 82, 89, 94	1 (0%)
1	B	266/275 (96%)	0.55	21 (7%)	12	9	71, 81, 88, 96	0
All	All	526/550 (95%)	0.53	44 (8%)	11	8	71, 81, 89, 96	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	ILE	6.9
1	B	74	ALA	6.5
1	B	152	VAL	5.9
1	B	326	PRO	5.7
1	A	165	LEU	5.5
1	B	327	THR	4.6
1	B	153	LEU	4.4
1	B	104	LEU	4.2
1	B	72	SER	4.0
1	B	331	PHE	3.9
1	A	137	HIS	3.8
1	A	104	LEU	3.8
1	A	88	PHE	3.4
1	B	149	ASN	3.3
1	B	128	ALA	3.3
1	A	126	ARG	3.2
1	A	128	ALA	3.1
1	A	150	THR	3.0
1	A	158	LEU	2.9
1	A	296	LEU	2.9
1	B	301	PHE	2.8
1	B	137	HIS	2.8
1	B	75	LEU	2.8
1	A	129	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	163	SER	2.7
1	B	227	HIS	2.7
1	B	162	ALA	2.7
1	B	311	ALA	2.7
1	A	121	THR	2.7
1	A	339	THR	2.6
1	A	79	SER	2.5
1	A	114	GLN	2.4
1	A	124	GLU	2.4
1	B	156	ALA	2.4
1	B	341	ILE	2.4
1	A	109	ASP	2.3
1	B	169	VAL	2.2
1	A	164	TYR	2.2
1	A	81	PHE	2.2
1	A	130	VAL	2.2
1	A	148	SER	2.1
1	A	318	ILE	2.1
1	A	144	LEU	2.1
1	B	212	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 carbohydrates 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.