Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2016 – 06:23 PM EDT

PDB ID	:	5IWN
Title	:	Bacterial sodium channel pore domain, high bromide
Authors	:	Shaya, D.; Findeisen, F.; Rohaim, A.; Minor, D.L.
Deposited on	:	2016-03-22
Resolution	:	3.75 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:

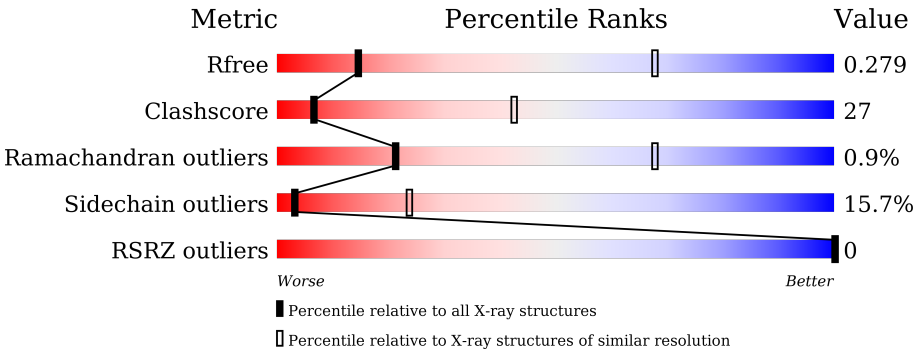
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 3.75 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	1268 (4.02-3.50)
Clashscore	102246	1407 (4.02-3.50)
Ramachandran outliers	100387	1346 (4.02-3.50)
Sidechain outliers	100360	1342 (4.02-3.50)
RSRZ outliers	91569	1276 (4.02-3.50)

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	152	47% 35% 9% 9%
1	B	152	40% 41% 9% 9%
1	C	152	39% 44% 8% 9%
1	D	152	36% 43% 12% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	A	301	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4502 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1124	742	181	195	6			
1	B	138	Total	C	N	O	S	0	1	0
			1126	745	180	195	6			
1	C	138	Total	C	N	O	S	0	0	0
			1122	742	178	196	6			
1	D	138	Total	C	N	O	S	0	0	0
			1128	745	181	196	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	-	expression tag	UNP Q0ABW0
A	138	PRO	-	expression tag	UNP Q0ABW0
A	139	SER	-	expression tag	UNP Q0ABW0
A	140	SER	-	expression tag	UNP Q0ABW0
A	141	PRO	-	expression tag	UNP Q0ABW0
A	142	SER	-	expression tag	UNP Q0ABW0
B	137	GLY	-	expression tag	UNP Q0ABW0
B	138	PRO	-	expression tag	UNP Q0ABW0
B	139	SER	-	expression tag	UNP Q0ABW0
B	140	SER	-	expression tag	UNP Q0ABW0
B	141	PRO	-	expression tag	UNP Q0ABW0
B	142	SER	-	expression tag	UNP Q0ABW0
C	137	GLY	-	expression tag	UNP Q0ABW0
C	138	PRO	-	expression tag	UNP Q0ABW0
C	139	SER	-	expression tag	UNP Q0ABW0
C	140	SER	-	expression tag	UNP Q0ABW0
C	141	PRO	-	expression tag	UNP Q0ABW0
C	142	SER	-	expression tag	UNP Q0ABW0
D	137	GLY	-	expression tag	UNP Q0ABW0
D	138	PRO	-	expression tag	UNP Q0ABW0
D	139	SER	-	expression tag	UNP Q0ABW0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	140	SER	-	expression tag	UNP Q0ABW0
D	141	PRO	-	expression tag	UNP Q0ABW0
D	142	SER	-	expression tag	UNP Q0ABW0

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

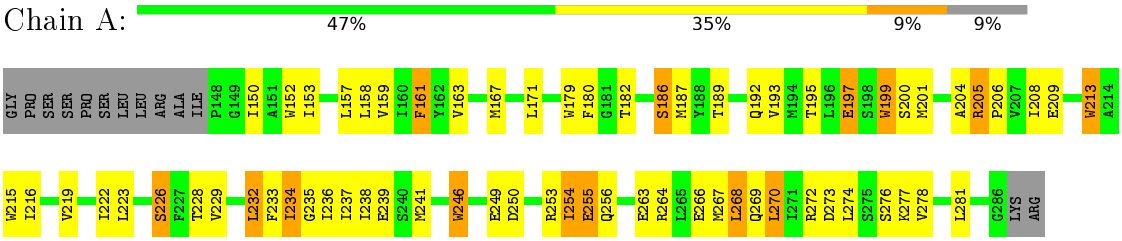
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Br 2 2	0	0

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.

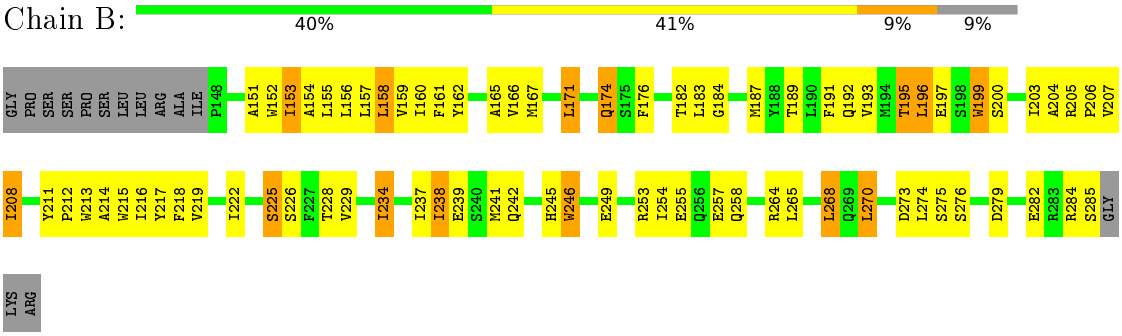
- Molecule 1: Ion transport protein

Chain A:



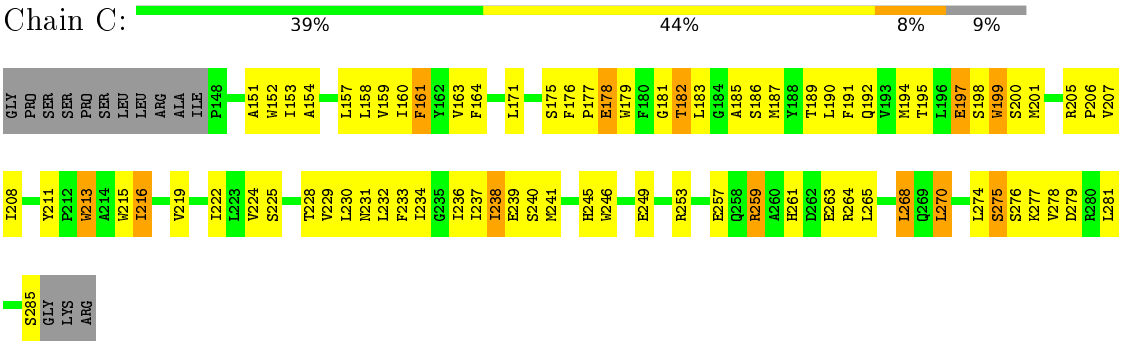
- Molecule 1: Ion transport protein

Chain B:



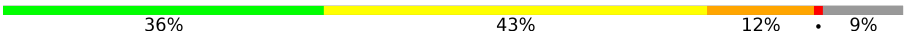
- Molecule 1: Ion transport protein

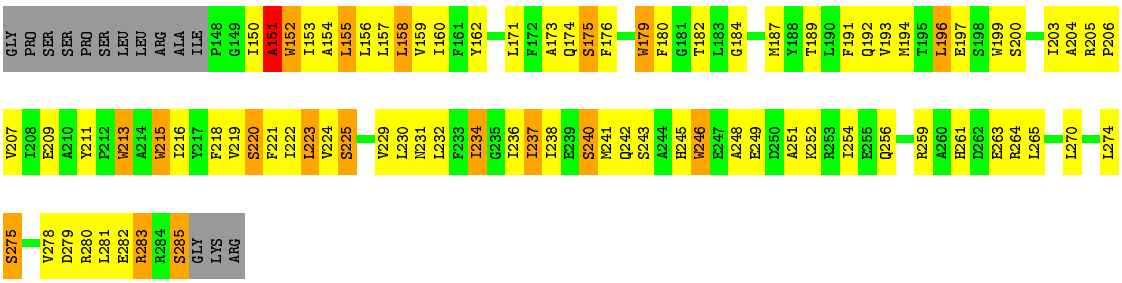
Chain C:



- Molecule 1: Ion transport protein

Chain D:




GLY
PRO
SER
SER
PRO
SER
LEU
LEU
ARG
ALA
ILE
P148
G149
I150
A151
W152
I153
A154
L155
L156
L157
L158
V159
I160
F161
Y162
L171
F172
A173
Q174
S175
F176
W179
F180
G181
T182
I183
G184
M187
Y188
T189
L190
F191
Q192
V193
H194
T195
L196
E197
S198
W199
S200
I203
A204
R205
P206
V207
I208
E209
A210
Y211
P212
W213
A214
W215
I216
Y217
F218
V219
S220
F221
I222
L223
V224
S225
V229
L230
N231
L232
F233
I234
G235
I236
I237
I238
E239
S240
M241
Q242
S243
A244
H245
W246
E247
A248
E249
D250
A251
K252
R253
I254
E255
Q256
R259
A260
H261
D262
E263
R264
L265
L270
L274
S275
V278
D279
R280
L281
E282
R283
R284
S285
GLY
LYS
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	157.40Å 160.87Å 167.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.75 14.98 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (15.00-3.75) 99.5 (14.98-3.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.26	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 3.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.228 , 0.280 0.222 , 0.279	Depositor DCC
R_{free} test set	1126 reflections (5.49%)	DCC
Wilson B-factor (Å^2)	144.1	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 101.9	EDS
Estimated twinning fraction	0.129 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Outliers	0 of 21634 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4502	wwPDB-VP
Average B, all atoms (Å^2)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: BR

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	0.70	3/1155 (0.3%)	0.78	1/1569 (0.1%)
1	B	0.70	3/1160 (0.3%)	0.77	1/1575 (0.1%)
1	C	0.76	4/1153 (0.3%)	0.81	0/1566
1	D	0.72	5/1159 (0.4%)	0.80	3/1573 (0.2%)
All	All	0.72	15/4627 (0.3%)	0.79	5/6283 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	199	TRP	CD2-CE2	6.69	1.49	1.41
1	C	152	TRP	CD2-CE2	5.74	1.48	1.41
1	D	179	TRP	CD2-CE2	5.50	1.48	1.41
1	A	152	TRP	CD2-CE2	5.50	1.48	1.41
1	C	213	TRP	CD2-CE2	5.43	1.47	1.41
1	C	246	TRP	CD2-CE2	5.41	1.47	1.41
1	D	152	TRP	CD2-CE2	5.26	1.47	1.41
1	B	246	TRP	CD2-CE2	5.22	1.47	1.41
1	A	246	TRP	CD2-CE2	5.14	1.47	1.41
1	D	213	TRP	CD2-CE2	5.12	1.47	1.41
1	B	152	TRP	CD2-CE2	5.11	1.47	1.41
1	B	199	TRP	CD2-CE2	5.10	1.47	1.41
1	D	246	TRP	CD2-CE2	5.10	1.47	1.41
1	D	215	TRP	CD2-CE2	5.07	1.47	1.41
1	A	213	TRP	CD2-CE2	5.07	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	D	196	LEU	CB-CG-CD1	-5.73	101.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	223	LEU	CA-CB-CG	-5.49	102.67	115.30
1	D	151	ALA	CB-CA-C	5.29	118.04	110.10
1	A	270	LEU	CB-CG-CD1	-5.02	102.47	111.00

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	1124	0	1111	71	0
1	B	1126	0	1119	61	0
1	C	1122	0	1112	85	0
1	D	1128	0	1123	78	0
2	A	2	0	0	6	0
All	All	4502	0	4465	244	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 27.

All (244) 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)
2:A:301:BR:BR	1:C:264:ARG:HD3	1.81	1.33
1:A:264:ARG:HD3	2:A:301:BR:BR	1.87	1.28
1:A:264:ARG:NE	2:A:301:BR:BR	2.25	1.23
1:A:264:ARG:CD	2:A:301:BR:BR	2.44	1.21
1:B:208:ILE:HD11	1:B:215:TRP:HB3	1.25	1.17
1:A:219:VAL:O	1:A:223:LEU:HG	1.60	1.01
2:A:301:BR:BR	1:C:264:ARG:CD	2.66	0.97
1:A:200:SER:O	1:A:205:ARG:HB2	1.66	0.94
1:A:180:PHE:HD1	1:A:186:SER:OG	1.50	0.94
1:A:267:MET:HG3	1:B:268:LEU:HD23	1.50	0.94
1:B:215:TRP:O	1:B:219:VAL:HG23	1.71	0.90
1:B:208:ILE:HD11	1:B:215:TRP:CB	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:PHE:HE2	1:C:194:MET:HE2	1.39	0.87
1:D:154:ALA:O	1:D:158:LEU:HD12	1.74	0.87
1:B:225:SER:O	1:B:229:VAL:HG23	1.75	0.87
1:B:274:LEU:HD21	1:C:274:LEU:HD23	1.55	0.87
1:A:263:GLU:OE1	1:B:264:ARG:HD2	1.76	0.86
1:C:192:GLN:HG3	1:D:200:SER:HB3	1.62	0.80
1:C:161:PHE:HE2	1:C:194:MET:CE	1.94	0.80
1:A:222:ILE:O	1:A:226:SER:HB2	1.81	0.80
1:D:200:SER:HA	1:D:204:ALA:HB3	1.62	0.79
1:C:264:ARG:HB2	1:C:264:ARG:HH21	1.48	0.79
1:A:267:MET:CG	1:B:268:LEU:HD23	2.13	0.79
1:C:263:GLU:OE1	1:D:264:ARG:NH2	2.15	0.79
1:C:245:HIS:CE1	1:D:246:TRP:HB3	2.18	0.78
1:A:171:LEU:HD22	1:A:213:TRP:HH2	1.47	0.78
1:A:269:GLN:OE1	1:A:269:GLN:HA	1.84	0.78
1:D:280:ARG:HA	1:D:283:ARG:HG2	1.65	0.77
1:D:151:ALA:HA	1:D:154:ALA:HB3	1.67	0.76
1:B:176:PHE:CZ	1:B:207:VAL:HA	2.21	0.75
1:A:180:PHE:HD1	1:A:186:SER:HG	0.76	0.74
1:A:195:THR:HB	1:B:196:LEU:HD13	1.69	0.74
1:C:237:ILE:O	1:C:240:SER:HB2	1.88	0.73
1:A:189:THR:O	1:A:193:VAL:HG23	1.88	0.72
1:C:264:ARG:NH2	1:C:264:ARG:HB2	2.05	0.72
1:A:246:TRP:O	1:A:250:ASP:HB2	1.89	0.71
1:D:173:ALA:HB2	1:D:180:PHE:O	1.90	0.71
1:B:258:GLN:HA	1:B:258:GLN:OE1	1.90	0.70
1:A:167:MET:O	1:A:171:LEU:HD12	1.91	0.70
1:C:197:GLU:OE1	1:D:200:SER:N	2.20	0.70
1:C:274:LEU:HD13	1:D:275:SER:HA	1.74	0.69
1:A:157:LEU:HD21	1:A:229:VAL:HG22	1.74	0.69
1:C:208:ILE:CD1	1:C:215:TRP:HB3	2.24	0.68
1:C:197:GLU:HG3	1:D:199:TRP:CD1	2.28	0.68
1:C:264:ARG:CB	1:C:264:ARG:HH21	2.05	0.68
1:D:171:LEU:HD13	1:D:213:TRP:CH2	2.29	0.68
1:D:171:LEU:HD13	1:D:213:TRP:HH2	1.56	0.68
1:B:197:GLU:HG3	1:C:199:TRP:CD1	2.28	0.68
1:C:197:GLU:OE2	1:C:198:SER:HB3	1.93	0.67
1:D:225:SER:O	1:D:229:VAL:HG23	1.95	0.67
1:A:277:LYS:HE2	1:B:279:ASP:HA	1.76	0.67
1:D:157:LEU:HA	1:D:160:ILE:HD12	1.77	0.66
1:C:208:ILE:HD11	1:C:215:TRP:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:PHE:O	1:A:237:ILE:HD12	1.96	0.66
1:A:274:LEU:HD13	1:B:275:SER:HA	1.78	0.66
1:D:150:ILE:C	1:D:152:TRP:H	2.00	0.65
1:C:211:TYR:HB3	1:C:213:TRP:NE1	2.11	0.65
1:B:189:THR:O	1:B:193:VAL:HG23	1.97	0.65
1:A:150:ILE:CD1	1:A:236:ILE:HG13	2.27	0.65
1:C:153:ILE:HD13	1:C:231:ASN:HB3	1.80	0.64
1:A:150:ILE:HD13	1:A:236:ILE:HG13	1.77	0.64
1:C:274:LEU:CD1	1:D:275:SER:HA	2.28	0.64
1:C:274:LEU:HD13	1:D:275:SER:OG	1.98	0.63
1:A:264:ARG:NH2	1:D:263:GLU:OE1	2.32	0.63
1:A:159:VAL:O	1:A:163:VAL:HG23	1.98	0.62
1:B:242:GLN:HA	1:B:246:TRP:HB2	1.83	0.61
1:B:192:GLN:NE2	1:B:197:GLU:O	2.33	0.61
1:C:161:PHE:CE2	1:C:194:MET:CE	2.82	0.59
1:D:216:ILE:O	1:D:220:SER:HB3	2.03	0.59
1:A:163:VAL:O	1:A:167:MET:HB2	2.03	0.59
1:D:150:ILE:HD12	1:D:151:ALA:N	2.17	0.59
1:A:205:ARG:NH1	1:D:192:GLN:OE1	2.35	0.59
1:A:204:ALA:O	1:A:208:ILE:HG13	2.02	0.59
1:C:192:GLN:HG3	1:D:200:SER:CB	2.32	0.59
1:A:215:TRP:O	1:A:219:VAL:HG23	2.02	0.58
1:A:234:ILE:HG22	1:A:235:GLY:N	2.19	0.58
1:C:277:LYS:HD3	1:D:279:ASP:HB3	1.85	0.58
1:A:153:ILE:CG2	1:A:232:LEU:HD12	2.33	0.58
1:A:237:ILE:HD13	1:D:237:ILE:HD11	1.86	0.58
1:B:218:PHE:O	1:B:222:ILE:HG12	2.04	0.57
1:C:197:GLU:OE2	1:C:198:SER:CB	2.52	0.57
1:A:267:MET:HG3	1:B:268:LEU:CD2	2.30	0.57
1:D:231:ASN:O	1:D:232:LEU:C	2.43	0.57
1:D:155:LEU:O	1:D:159:VAL:HG23	2.05	0.57
1:B:205:ARG:HB3	1:B:206:PRO:HD3	1.86	0.56
1:B:154:ALA:O	1:B:158:LEU:HD22	2.05	0.56
1:C:163:VAL:HG12	1:C:164:PHE:N	2.19	0.56
1:A:171:LEU:HD22	1:A:213:TRP:CH2	2.36	0.56
1:C:195:THR:HB	1:D:196:LEU:HD13	1.88	0.55
1:A:246:TRP:O	1:A:250:ASP:CB	2.53	0.55
2:A:301:BR:BR	1:C:264:ARG:NE	2.95	0.55
1:A:192:GLN:OE1	1:B:205:ARG:NH2	2.39	0.55
1:B:208:ILE:CD1	1:B:215:TRP:HB3	2.17	0.54
1:C:237:ILE:HG13	1:D:234:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:SER:C	1:C:177:PRO:HD3	2.29	0.53
1:B:211:TYR:O	1:B:213:TRP:N	2.42	0.53
1:C:182:THR:HG23	1:C:185:ALA:HB2	1.91	0.53
1:A:153:ILE:HG23	1:A:232:LEU:CD1	2.40	0.52
1:A:246:TRP:CZ3	1:D:245:HIS:HB2	2.43	0.52
1:C:190:LEU:O	1:C:194:MET:HB2	2.10	0.52
1:D:281:LEU:O	1:D:285:SER:HB2	2.09	0.52
1:A:237:ILE:HA	1:B:234:ILE:HD11	1.90	0.52
1:A:269:GLN:OE1	1:A:269:GLN:CA	2.57	0.52
1:C:276:SER:O	1:C:279:ASP:N	2.42	0.52
1:B:200:SER:HA	1:B:204:ALA:HB3	1.92	0.52
1:C:176:PHE:CZ	1:C:207:VAL:HA	2.45	0.52
1:D:150:ILE:C	1:D:152:TRP:N	2.62	0.51
1:A:268:LEU:HD11	1:A:272:ARG:NH2	2.25	0.51
1:B:167:MET:O	1:B:171:LEU:HG	2.10	0.51
1:C:161:PHE:HE1	1:C:187:MET:HA	1.75	0.51
1:A:237:ILE:HG13	1:B:234:ILE:HD11	1.92	0.51
1:C:151:ALA:HA	1:C:154:ALA:HB3	1.93	0.51
1:D:205:ARG:N	1:D:206:PRO:HD2	2.25	0.51
1:D:238:ILE:HA	1:D:241:MET:HE2	1.92	0.51
1:D:196:LEU:HD22	1:D:199:TRP:CD1	2.46	0.51
1:C:238:ILE:HG22	1:C:239:GLU:N	2.26	0.51
1:C:160:ILE:HD13	1:C:224:VAL:CG1	2.41	0.50
1:A:193:VAL:HG13	1:A:199:TRP:HB2	1.93	0.50
1:D:153:ILE:O	1:D:156:LEU:N	2.45	0.50
1:C:208:ILE:HD11	1:C:215:TRP:CA	2.41	0.50
1:D:236:ILE:O	1:D:240:SER:HB2	2.10	0.50
1:C:161:PHE:CE2	1:C:194:MET:HE2	2.31	0.50
1:A:205:ARG:N	1:A:206:PRO:CD	2.75	0.49
1:D:150:ILE:O	1:D:152:TRP:N	2.45	0.49
1:D:176:PHE:CZ	1:D:207:VAL:HA	2.46	0.49
1:C:161:PHE:CE2	1:C:194:MET:HE1	2.48	0.49
1:A:153:ILE:CG2	1:A:232:LEU:CD1	2.90	0.49
1:B:215:TRP:CE2	1:B:216:ILE:HG13	2.48	0.49
1:D:151:ALA:HA	1:D:154:ALA:CB	2.41	0.49
1:A:270:LEU:O	1:A:273:ASP:HB2	2.12	0.49
1:A:197:GLU:HG3	1:B:199:TRP:CD1	2.48	0.49
1:C:278:VAL:HG23	1:D:278:VAL:HG11	1.94	0.49
1:B:191:PHE:O	1:B:195:THR:HG23	2.13	0.48
1:D:221:PHE:O	1:D:225:SER:HB3	2.13	0.48
1:A:195:THR:HB	1:B:196:LEU:CD1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:PHE:CE2	1:B:207:VAL:HA	2.48	0.48
1:B:156:LEU:O	1:B:159:VAL:HB	2.14	0.48
1:C:275:SER:O	1:C:279:ASP:HB2	2.12	0.48
1:D:191:PHE:HA	1:D:194:MET:HB2	1.96	0.48
1:D:224:VAL:HG12	1:D:225:SER:N	2.28	0.48
1:C:151:ALA:HA	1:C:154:ALA:CB	2.42	0.47
1:B:237:ILE:CD1	1:C:237:ILE:HG21	2.44	0.47
1:C:208:ILE:HD11	1:C:215:TRP:CB	2.44	0.47
1:A:157:LEU:CD2	1:A:229:VAL:HG22	2.42	0.47
1:B:199:TRP:CZ3	1:B:200:SER:HB2	2.50	0.47
1:D:251:ALA:O	1:D:254:ILE:HG22	2.15	0.47
1:C:233:PHE:CD2	1:D:230:LEU:HD11	2.49	0.47
1:A:150:ILE:O	1:A:153:ILE:HG22	2.14	0.47
1:A:281:LEU:HD23	1:D:281:LEU:CD1	2.45	0.47
1:B:157:LEU:HA	1:B:160:ILE:HD12	1.96	0.47
1:B:211:TYR:C	1:B:213:TRP:H	2.18	0.47
1:C:205:ARG:CB	1:C:206:PRO:HD3	2.45	0.47
1:A:278:VAL:HG21	1:D:274:LEU:HD11	1.97	0.47
1:A:200:SER:HA	1:A:204:ALA:HB3	1.96	0.46
1:C:182:THR:OG1	1:C:183:LEU:N	2.48	0.46
1:C:232:LEU:O	1:C:236:ILE:HB	2.15	0.46
1:D:153:ILE:HD11	1:D:232:LEU:HA	1.96	0.46
1:A:241:MET:HG2	1:B:241:MET:HE1	1.97	0.46
1:C:234:ILE:O	1:C:237:ILE:N	2.47	0.46
1:C:160:ILE:HG21	1:C:224:VAL:HG12	1.96	0.46
1:D:248:ALA:O	1:D:252:LYS:HE3	2.14	0.46
1:B:156:LEU:O	1:B:160:ILE:HG13	2.16	0.46
1:C:205:ARG:CB	1:C:206:PRO:CD	2.94	0.46
1:D:184:GLY:HA2	1:D:187:MET:HE3	1.97	0.46
1:C:215:TRP:CE3	1:C:216:ILE:N	2.83	0.46
1:D:189:THR:O	1:D:193:VAL:HG23	2.16	0.46
1:B:245:HIS:NE2	1:B:249:GLU:OE1	2.49	0.46
1:C:191:PHE:O	1:C:195:THR:HG23	2.16	0.46
1:C:233:PHE:HD2	1:D:230:LEU:HD11	1.80	0.46
1:B:157:LEU:HB2	1:B:228:THR:HG21	1.98	0.46
1:A:179:TRP:HD1	1:B:205:ARG:NH1	2.14	0.46
1:C:191:PHE:CE2	1:D:219:VAL:HG22	2.50	0.46
1:B:162:TYR:O	1:B:166:VAL:HG23	2.16	0.45
1:D:223:LEU:HD23	1:D:223:LEU:HA	1.68	0.45
1:D:218:PHE:O	1:D:222:ILE:HG13	2.17	0.45
1:A:205:ARG:N	1:A:206:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ALA:O	1:B:217:TYR:HB3	2.17	0.45
1:D:162:TYR:C	1:D:162:TYR:CD1	2.90	0.45
1:A:238:ILE:HG22	1:A:239:GLU:N	2.31	0.45
1:C:177:PRO:HD2	1:C:178:GLU:OE1	2.16	0.45
1:C:259:ARG:HE	1:C:259:ARG:HB2	1.51	0.45
1:D:232:LEU:HD23	1:D:236:ILE:HD12	1.97	0.45
1:D:173:ALA:CB	1:D:180:PHE:O	2.62	0.45
1:C:177:PRO:O	1:C:181:GLY:HA3	2.17	0.45
1:C:277:LYS:CD	1:D:279:ASP:HB3	2.46	0.45
1:C:176:PHE:N	1:C:177:PRO:HD3	2.32	0.44
1:B:153:ILE:HG13	1:B:153:ILE:H	1.60	0.44
1:B:160:ILE:H	1:B:160:ILE:HG13	1.57	0.44
1:B:174:GLN:HE21	1:B:174:GLN:HB3	1.57	0.44
1:C:261:HIS:CD2	1:C:261:HIS:C	2.90	0.44
1:A:157:LEU:HD13	1:A:228:THR:HB	2.00	0.43
1:C:171:LEU:HD22	1:C:213:TRP:CH2	2.54	0.43
1:C:257:GLU:OE2	1:C:264:ARG:NH1	2.51	0.43
1:C:178:GLU:CD	1:C:178:GLU:H	2.21	0.43
1:C:225:SER:O	1:C:229:VAL:HG23	2.18	0.43
1:C:263:GLU:OE2	1:D:261:HIS:ND1	2.51	0.43
1:C:245:HIS:HE1	1:D:246:TRP:HB3	1.73	0.43
1:D:215:TRP:CE2	1:D:216:ILE:HG12	2.53	0.43
1:C:241:MET:SD	1:D:241:MET:HE3	2.58	0.42
1:B:203:ILE:O	1:B:207:VAL:HG23	2.18	0.42
1:C:268:LEU:HD13	1:C:268:LEU:HA	1.55	0.42
1:C:276:SER:O	1:C:277:LYS:C	2.57	0.42
1:B:284:ARG:O	1:B:285:SER:C	2.57	0.42
1:D:231:ASN:O	1:D:234:ILE:N	2.53	0.42
1:A:246:TRP:HB3	1:D:245:HIS:CE1	2.53	0.42
1:A:205:ARG:O	1:A:209:GLU:HG3	2.20	0.42
1:A:254:ILE:HG22	1:A:255:GLU:N	2.34	0.42
1:B:265:LEU:HD12	1:B:265:LEU:HA	1.79	0.42
1:A:161:PHE:HB3	1:A:187:MET:CE	2.50	0.42
1:C:201:MET:HE1	1:C:205:ARG:NH1	2.34	0.42
1:D:150:ILE:HD12	1:D:151:ALA:H	1.81	0.42
1:B:197:GLU:HG3	1:C:199:TRP:HD1	1.82	0.42
1:C:281:LEU:HG	1:D:282:GLU:HG3	2.02	0.42
1:D:196:LEU:HD23	1:D:196:LEU:HA	1.71	0.42
1:A:205:ARG:NH2	1:D:179:TRP:HD1	2.17	0.42
1:A:199:TRP:CD1	1:D:197:GLU:HG3	2.55	0.42
1:A:215:TRP:CG	1:A:216:ILE:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:PHE:O	1:B:165:ALA:HB2	2.19	0.42
1:A:234:ILE:CG2	1:A:235:GLY:N	2.83	0.42
1:B:268:LEU:HA	1:B:268:LEU:HD22	1.66	0.42
1:D:203:ILE:O	1:D:206:PRO:HG2	2.20	0.41
1:B:274:LEU:HD21	1:C:274:LEU:CD2	2.39	0.41
1:B:192:GLN:OE1	1:C:200:SER:HB3	2.20	0.41
1:C:157:LEU:HD23	1:C:228:THR:HB	2.02	0.41
1:D:280:ARG:O	1:D:280:ARG:HG3	2.21	0.41
1:A:266:GLU:O	1:A:269:GLN:HB3	2.20	0.41
1:B:184:GLY:HA2	1:B:187:MET:HG3	2.00	0.41
1:C:176:PHE:CE2	1:C:207:VAL:HG22	2.54	0.41
1:A:256:GLN:CD	1:B:257:GLU:HG3	2.40	0.41
1:B:155:LEU:O	1:B:159:VAL:HG23	2.21	0.41
1:D:175:SER:HG	1:D:211:TYR:HH	1.69	0.41
1:C:278:VAL:CG1	1:C:278:VAL:O	2.68	0.41
1:D:184:GLY:HA2	1:D:187:MET:CE	2.50	0.41
1:A:180:PHE:CD1	1:A:186:SER:OG	2.42	0.41
1:A:205:ARG:H	1:A:206:PRO:HD2	1.86	0.41
1:B:238:ILE:HG22	1:B:239:GLU:N	2.36	0.41
1:D:281:LEU:HD23	1:D:281:LEU:HA	1.69	0.41
1:C:186:SER:O	1:C:187:MET:C	2.59	0.41
1:D:270:LEU:HD23	1:D:270:LEU:HA	1.95	0.41
1:A:215:TRP:CE2	1:A:216:ILE:HG13	2.56	0.40
1:C:179:TRP:HB3	1:C:189:THR:HG21	2.04	0.40
1:D:215:TRP:O	1:D:216:ILE:C	2.59	0.40
1:B:270:LEU:HA	1:B:270:LEU:HD22	1.76	0.40
1:C:270:LEU:HD23	1:C:270:LEU:H	1.86	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	137/152 (90%)	117 (85%)	19 (14%)	1 (1%)	26 72
1	B	137/152 (90%)	119 (87%)	16 (12%)	2 (2%)	13 59
1	C	136/152 (90%)	114 (84%)	21 (15%)	1 (1%)	26 72
1	D	136/152 (90%)	115 (85%)	20 (15%)	1 (1%)	26 72
All	All	546/608 (90%)	465 (85%)	76 (14%)	5 (1%)	21 68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	151	ALA
1	A	199	TRP
1	B	151	ALA
1	B	212	PRO
1	C	216	ILE

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	117/131 (89%)	101 (86%)	16 (14%)	4 30
1	B	118/131 (90%)	98 (83%)	20 (17%)	2 19
1	C	118/131 (90%)	100 (85%)	18 (15%)	3 25
1	D	119/131 (91%)	99 (83%)	20 (17%)	2 19
All	All	472/524 (90%)	398 (84%)	74 (16%)	3 24

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	LEU
1	A	161	PHE
1	A	182	THR
1	A	186	SER
1	A	197	GLU
1	A	201	MET

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Mol	Chain	Res	Type
1	A	205	ARG
1	A	226	SER
1	A	232	LEU
1	A	234	ILE
1	A	249	GLU
1	A	253	ARG
1	A	254	ILE
1	A	255	GLU
1	A	268	LEU
1	A	276	SER
1	B	153	ILE
1	B	158	LEU
1	B	171	LEU
1	B	174	GLN
1	B	182	THR
1	B	183	LEU
1	B	195	THR
1	B	208	ILE
1	B	225	SER
1	B	226	SER
1	B	234	ILE
1	B	238	ILE
1	B	253	ARG
1	B	254	ILE
1	B	255	GLU
1	B	268	LEU
1	B	270	LEU
1	B	273	ASP
1	B	276	SER
1	B	282	GLU
1	C	158	LEU
1	C	159	VAL
1	C	161	PHE
1	C	178	GLU
1	C	182	THR
1	C	197	GLU
1	C	219	VAL
1	C	222	ILE
1	C	230	LEU
1	C	238	ILE
1	C	249	GLU
1	C	253	ARG

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Mol	Chain	Res	Type
1	C	259	ARG
1	C	265	LEU
1	C	268	LEU
1	C	270	LEU
1	C	275	SER
1	C	285	SER
1	D	155	LEU
1	D	158	LEU
1	D	174	GLN
1	D	175	SER
1	D	182	THR
1	D	209	GLU
1	D	220	SER
1	D	225	SER
1	D	234	ILE
1	D	237	ILE
1	D	240	SER
1	D	242	GLN
1	D	243	SER
1	D	249	GLU
1	D	256	GLN
1	D	259	ARG
1	D	265	LEU
1	D	275	SER
1	D	283	ARG
1	D	285	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	B	174	GLN
1	B	231	ASN
1	B	242	GLN
1	C	242	GLN
1	C	245	HIS
1	D	245	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

Of 2 ligands modelled in this entry, 2 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	139/152 (91%)	-0.81	0	100	100	125, 169, 207, 233	0
1	B	138/152 (90%)	-0.79	0	100	100	130, 171, 213, 242	0
1	C	138/152 (90%)	-0.76	0	100	100	117, 165, 214, 258	0
1	D	138/152 (90%)	-0.78	0	100	100	115, 160, 203, 246	0
All	All	553/608 (90%)	-0.78	0	100	100	115, 166, 211, 258	0

There are no RSRZ outliers to report.

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	BR	A	301	1/1	0.92	0.50	-	178,178,178,178	0
2	BR	A	302	1/1	0.92	0.31	-	195,195,195,195	0

6.5 Other polymers (i)

There are no such residues in this entry.