Full wwPDB X-ray Structure Validation Report (i)

Mar 20, 2016 – 06:16 PM EDT

PDB ID	:	5HK6
Title	:	Bacterial sodium channel neck 3G mutant, SAD
Authors	:	Rohaim, A.; Minor, D.L.
Deposited on	:	2016-01-13
Resolution	:	5.50 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:

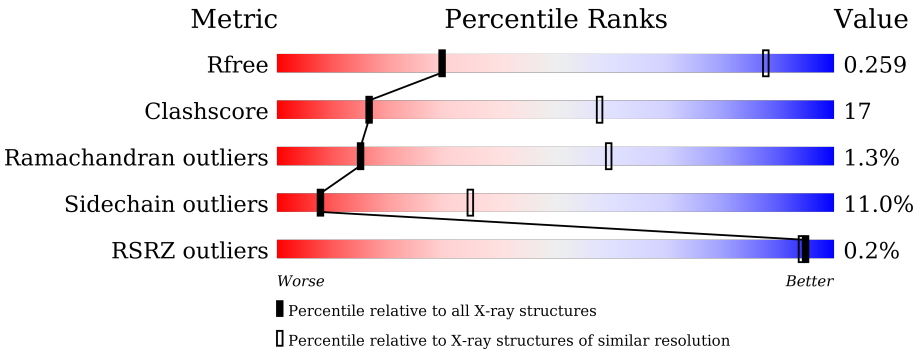
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 5.50 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	1015 (7.38-3.62)
Clashscore	102246	1020 (7.10-3.70)
Ramachandran outliers	100387	1014 (7.36-3.64)
Sidechain outliers	100360	1013 (7.38-3.62)
RSRZ outliers	91569	1014 (7.38-3.62)

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	53% 22% 5% • 18%
1	B	152	% 52% 17% 6% 25%
1	C	152	55% 20% 5% • 18%
1	D	152	59% 15% 5% • 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3701 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	125	Total	C	N	O	Se	0	0	0
			956	640	143	167	6			
1	B	114	Total	C	N	O	Se	0	0	0
			898	605	135	152	6			
1	C	124	Total	C	N	O	Se	0	0	1
			920	618	139	157	6			
1	D	123	Total	C	N	O	Se	0	0	0
			923	623	139	155	6			

There are 36 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
A	248	GLY	ALA	engineered mutation	UNP Q0ABW0
A	249	GLY	GLU	engineered mutation	UNP Q0ABW0
A	250	GLY	ASP	engineered mutation	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
B	248	GLY	ALA	engineered mutation	UNP Q0ABW0
B	249	GLY	GLU	engineered mutation	UNP Q0ABW0
B	250	GLY	ASP	engineered mutation	UNP Q0ABW0
C	137	GLY	-	expression tag	UNP Q0ABW0
C	138	PRO	-	expression tag	UNP Q0ABW0
C	139	SER	-	expression tag	UNP Q0ABW0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	140	SER	-	expression tag	UNP Q0ABW0
C	141	PRO	-	expression tag	UNP Q0ABW0
C	142	SER	-	expression tag	UNP Q0ABW0
C	248	GLY	ALA	engineered mutation	UNP Q0ABW0
C	249	GLY	GLU	engineered mutation	UNP Q0ABW0
C	250	GLY	ASP	engineered mutation	UNP Q0ABW0
D	137	GLY	-	expression tag	UNP Q0ABW0
D	138	PRO	-	expression tag	UNP Q0ABW0
D	139	SER	-	expression tag	UNP Q0ABW0
D	140	SER	-	expression tag	UNP Q0ABW0
D	141	PRO	-	expression tag	UNP Q0ABW0
D	142	SER	-	expression tag	UNP Q0ABW0
D	248	GLY	ALA	engineered mutation	UNP Q0ABW0
D	249	GLY	GLU	engineered mutation	UNP Q0ABW0
D	250	GLY	ASP	engineered mutation	UNP Q0ABW0

- Molecule 2 is water.

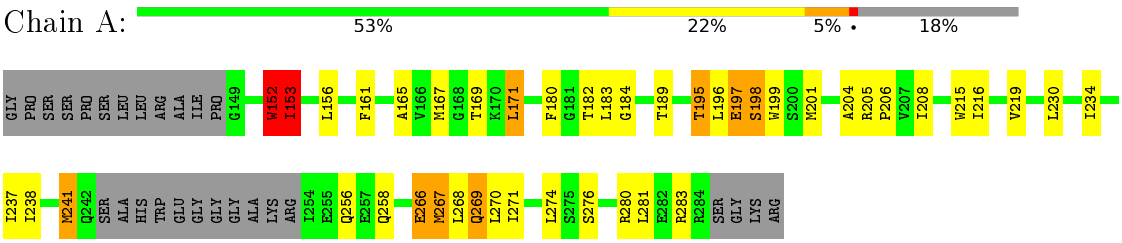
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O 1 1	0	0
2	C	2	Total O 2 2	0	0
2	D	1	Total O 1 1	0	0

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.

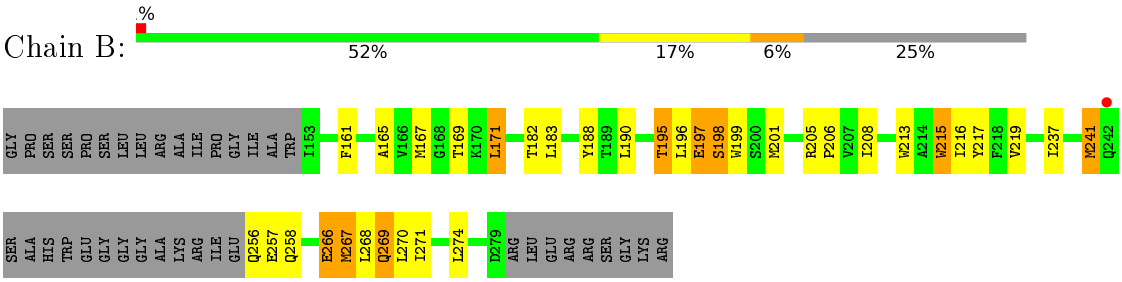
- Molecule 1: Ion transport protein

Chain A:



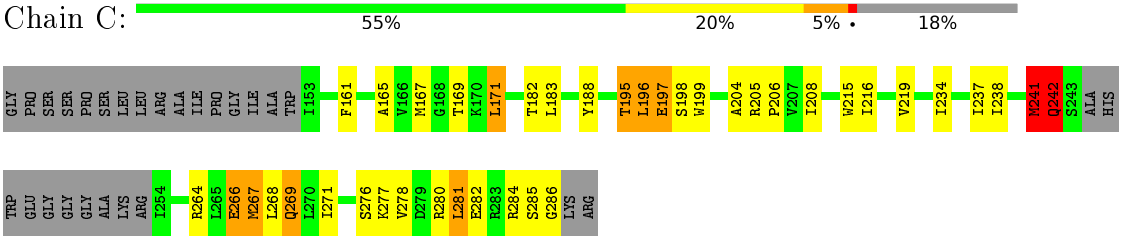
- Molecule 1: Ion transport protein

Chain B:



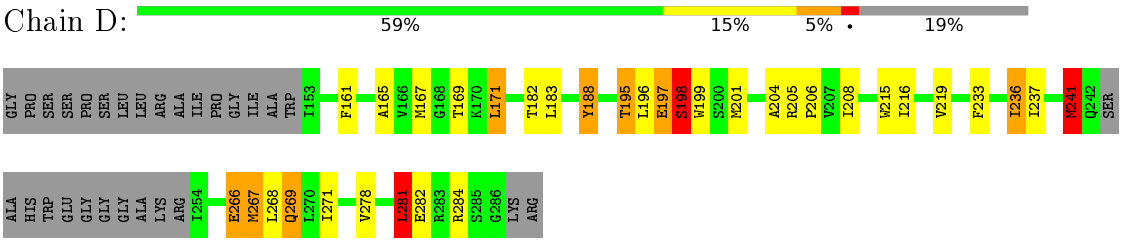
- Molecule 1: Ion transport protein

Chain C:



- Molecule 1: Ion transport protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	144.35Å 150.19Å 167.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 5.50 14.96 – 5.50	Depositor EDS
% Data completeness (in resolution range)	94.4 (15.00-5.50) 100.0 (14.96-5.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 5.39Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.256 , 0.264 0.259 , 0.259	Depositor DCC
R_{free} test set	297 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	371.2	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.14 , 155.1	EDS
Estimated twinning fraction	0.109 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Outliers	2 of 5848 reflections (0.034%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3701	wwPDB-VP
Average B, all atoms (Å^2)	294.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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

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	0.52	0/974	0.81	3/1319 (0.2%)
1	B	0.55	1/916 (0.1%)	0.73	1/1238 (0.1%)
1	C	0.49	0/936	0.85	2/1268 (0.2%)
1	D	0.55	0/941	0.74	1/1276 (0.1%)
All	All	0.53	1/3767 (0.0%)	0.78	7/5101 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	4
1	D	0	2
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	213	TRP	CB-CG	5.04	1.59	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	242	GLN	N-CA-C	12.05	143.54	111.00
1	C	242	GLN	CB-CA-C	-11.57	87.25	110.40
1	A	152	TRP	CB-CA-C	-9.06	92.28	110.40
1	A	153	ILE	N-CA-CB	-8.71	90.77	110.80
1	A	153	ILE	N-CA-C	5.31	125.33	111.00
1	D	241	MSE	CB-CA-C	-5.12	100.16	110.40
1	B	215	TRP	CB-CA-C	-5.08	100.24	110.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	TRP	Peptide
1	A	195	THR	Peptide
1	B	195	THR	Peptide
1	C	195	THR	Peptide
1	C	241	MSE	Peptide
1	C	242	GLN	Mainchain
1	C	281	LEU	Peptide
1	D	195	THR	Peptide
1	D	281	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	956	0	910	33	0
1	B	898	0	880	33	0
1	C	920	0	875	45	0
1	D	923	0	877	39	0
2	B	1	0	0	0	0
2	C	2	0	0	1	0
2	D	1	0	0	0	0
All	All	3701	0	3542	120	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 17.

All (120) 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:C:241:MSE:HB3	1:C:242:GLN:CB	1.80	1.10
1:C:241:MSE:CB	1:C:242:GLN:CB	2.47	0.93
1:C:197:GLU:OE1	1:C:198:SER:OG	1.93	0.87
1:A:197:GLU:OE1	1:A:198:SER:OG	1.96	0.84
1:A:234:ILE:HD11	1:D:237:ILE:HA	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:GLU:OE1	1:D:198:SER:OG	2.00	0.79
1:C:277:LYS:CB	2:C:301:HOH:O	2.35	0.72
1:C:188:TYR:OH	1:D:204:ALA:HB3	1.90	0.72
1:A:198:SER:HB2	1:B:201:MSE:HG3	1.72	0.71
1:C:282:GLU:O	1:C:285:SER:CB	2.41	0.68
1:C:167:MSE:O	1:C:171:LEU:HD13	1.94	0.68
1:A:201:MSE:HG3	1:D:198:SER:HB2	1.76	0.66
1:A:167:MSE:O	1:A:171:LEU:HD13	1.95	0.66
1:B:167:MSE:O	1:B:171:LEU:HD13	1.96	0.66
1:D:167:MSE:O	1:D:171:LEU:HD13	1.96	0.65
1:B:267:MSE:SE	1:C:267:MSE:HB3	2.46	0.65
1:B:215:TRP:C	1:B:215:TRP:CD1	2.69	0.64
1:C:215:TRP:C	1:C:215:TRP:CD1	2.70	0.64
1:C:182:THR:HG22	1:C:183:LEU:HD22	1.80	0.64
1:A:215:TRP:C	1:A:215:TRP:CD1	2.72	0.63
1:D:182:THR:HG22	1:D:183:LEU:HD22	1.81	0.63
1:B:182:THR:HG22	1:B:183:LEU:HD22	1.80	0.62
1:A:182:THR:HG22	1:A:183:LEU:HD22	1.81	0.61
1:B:237:ILE:HA	1:C:234:ILE:HD11	1.83	0.61
1:B:241:MSE:HE3	1:C:238:ILE:HG23	1.83	0.61
1:C:266:GLU:HA	1:C:269:GLN:HB2	1.84	0.60
1:D:215:TRP:C	1:D:215:TRP:CD1	2.75	0.59
1:D:266:GLU:HA	1:D:269:GLN:HB2	1.85	0.57
1:A:274:LEU:HD22	1:B:271:ILE:HG23	1.87	0.57
1:A:197:GLU:CD	1:A:198:SER:OG	2.43	0.57
1:A:266:GLU:HA	1:A:269:GLN:HB2	1.87	0.56
1:B:270:LEU:HG	1:C:271:ILE:HG21	1.86	0.56
1:D:183:LEU:HD22	1:D:183:LEU:H	1.70	0.56
1:B:266:GLU:HA	1:B:269:GLN:HB2	1.87	0.56
1:C:267:MSE:HG2	1:D:268:LEU:HD21	1.88	0.55
1:C:241:MSE:HB2	1:C:242:GLN:CB	2.35	0.54
1:A:270:LEU:HD23	1:B:268:LEU:HD23	1.88	0.54
1:A:184:GLY:HA2	1:B:215:TRP:CH2	2.43	0.54
1:C:165:ALA:O	1:C:169:THR:OG1	2.24	0.54
1:B:274:LEU:CD1	1:C:278:VAL:HG21	2.38	0.53
1:D:281:LEU:HD12	1:D:284:ARG:CB	2.38	0.53
1:C:285:SER:O	1:C:286:GLY:C	2.46	0.52
1:A:204:ALA:HB3	1:D:188:TYR:OH	2.09	0.52
1:A:234:ILE:HD11	1:D:237:ILE:CA	2.36	0.52
1:C:197:GLU:O	1:C:198:SER:C	2.48	0.52
1:A:184:GLY:HA2	1:B:215:TRP:HH2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LEU:O	1:A:271:ILE:N	2.43	0.52
1:C:188:TYR:OH	1:D:204:ALA:CB	2.58	0.51
1:B:183:LEU:HD22	1:B:183:LEU:H	1.76	0.51
1:B:188:TYR:OH	1:C:204:ALA:HB3	2.10	0.51
1:C:268:LEU:O	1:C:271:ILE:N	2.44	0.51
1:B:241:MSE:HE1	1:C:242:GLN:O	2.12	0.50
1:A:196:LEU:HA	1:A:199:TRP:CD1	2.47	0.49
1:D:268:LEU:O	1:D:271:ILE:N	2.45	0.49
1:B:196:LEU:HA	1:B:199:TRP:CD1	2.48	0.48
1:C:208:ILE:O	1:C:208:ILE:HG22	2.13	0.48
1:B:268:LEU:O	1:B:271:ILE:N	2.46	0.48
1:A:230:LEU:HD21	1:D:236:ILE:HG13	1.96	0.48
1:A:208:ILE:O	1:A:208:ILE:HG22	2.14	0.48
1:C:215:TRP:O	1:C:215:TRP:CD1	2.66	0.47
1:A:276:SER:O	1:A:280:ARG:CB	2.62	0.47
1:B:208:ILE:O	1:B:208:ILE:HG22	2.14	0.47
1:C:196:LEU:HA	1:C:199:TRP:CD1	2.49	0.47
1:C:183:LEU:HD22	1:C:183:LEU:H	1.80	0.47
1:D:208:ILE:HG22	1:D:208:ILE:O	2.14	0.47
1:A:153:ILE:HA	1:A:156:LEU:HB3	1.97	0.47
1:D:196:LEU:HA	1:D:199:TRP:CD1	2.50	0.46
1:D:188:TYR:HD1	1:D:188:TYR:O	1.99	0.46
1:A:267:MSE:HA	1:B:268:LEU:HD21	1.97	0.46
1:D:197:GLU:O	1:D:198:SER:C	2.55	0.46
1:C:276:SER:O	1:C:280:ARG:CB	2.64	0.45
1:D:188:TYR:C	1:D:188:TYR:CD1	2.89	0.45
1:C:281:LEU:HD22	1:D:282:GLU:CB	2.45	0.45
1:C:281:LEU:HA	1:C:284:ARG:CB	2.47	0.45
1:A:201:MSE:HG3	1:D:198:SER:CB	2.46	0.45
1:A:216:ILE:O	1:A:219:VAL:N	2.49	0.45
1:B:205:ARG:HB2	1:B:206:PRO:HD3	1.97	0.45
1:D:278:VAL:O	1:D:282:GLU:N	2.49	0.45
1:C:195:THR:O	1:C:197:GLU:N	2.50	0.45
1:C:197:GLU:CD	1:C:198:SER:OG	2.54	0.45
1:D:197:GLU:CD	1:D:198:SER:OG	2.53	0.45
1:A:198:SER:N	1:D:197:GLU:HG3	2.32	0.44
1:D:165:ALA:O	1:D:169:THR:OG1	2.23	0.44
1:D:183:LEU:HD22	1:D:183:LEU:N	2.32	0.44
1:A:197:GLU:O	1:A:199:TRP:N	2.51	0.44
1:C:183:LEU:N	1:C:183:LEU:HD22	2.33	0.43
1:A:267:MSE:HB3	1:D:267:MSE:SE	2.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:THR:O	1:B:197:GLU:N	2.51	0.43
1:C:198:SER:HB2	1:D:201:MSE:HG3	2.01	0.43
1:D:237:ILE:O	1:D:241:MSE:HG3	2.18	0.43
1:B:183:LEU:HD22	1:B:183:LEU:N	2.33	0.43
1:D:205:ARG:HB2	1:D:206:PRO:HD3	2.00	0.43
1:C:216:ILE:O	1:C:219:VAL:N	2.52	0.42
1:D:195:THR:O	1:D:197:GLU:N	2.53	0.42
1:C:182:THR:HG22	1:C:183:LEU:H	1.84	0.42
1:C:237:ILE:O	1:C:241:MSE:HG3	2.19	0.42
1:D:182:THR:HG22	1:D:183:LEU:H	1.84	0.42
1:A:238:ILE:HG23	1:D:241:MSE:HE3	2.03	0.41
1:B:182:THR:HG22	1:B:183:LEU:H	1.84	0.41
1:B:197:GLU:O	1:B:198:SER:C	2.59	0.41
1:B:165:ALA:O	1:B:169:THR:OG1	2.24	0.41
1:C:264:ARG:HA	1:C:267:MSE:HG3	2.03	0.41
1:C:278:VAL:O	1:C:282:GLU:CB	2.68	0.41
1:B:237:ILE:O	1:B:241:MSE:HG3	2.21	0.41
1:B:267:MSE:HE1	1:C:267:MSE:HE2	2.03	0.41
1:C:197:GLU:HG2	1:D:198:SER:H	1.85	0.41
1:A:180:PHE:CE2	1:A:189:THR:HG21	2.56	0.41
1:A:195:THR:O	1:A:197:GLU:N	2.54	0.41
1:B:190:LEU:HD21	1:B:217:TYR:OH	2.21	0.41
1:B:270:LEU:HD21	1:C:271:ILE:CG2	2.50	0.41
1:C:266:GLU:HA	1:C:269:GLN:CB	2.49	0.41
1:A:237:ILE:O	1:A:241:MSE:HG3	2.21	0.41
1:B:216:ILE:O	1:B:219:VAL:N	2.54	0.40
1:C:205:ARG:HB2	1:C:206:PRO:HD3	2.03	0.40
1:D:197:GLU:O	1:D:199:TRP:N	2.55	0.40
1:D:197:GLU:CD	1:D:198:SER:HG	2.24	0.40
1:A:165:ALA:O	1:A:169:THR:OG1	2.24	0.40
1:A:205:ARG:HB2	1:A:206:PRO:HD3	2.02	0.40
1:D:216:ILE:O	1:D:219:VAL:N	2.55	0.40
1:B:216:ILE:O	1:B:217:TYR:C	2.60	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	121/152 (80%)	99 (82%)	18 (15%)	4 (3%)	5 40
1	B	110/152 (72%)	94 (86%)	16 (14%)	0	100 100
1	C	120/152 (79%)	103 (86%)	16 (13%)	1 (1%)	24 69
1	D	119/152 (78%)	103 (87%)	15 (13%)	1 (1%)	24 69
All	All	470/608 (77%)	399 (85%)	65 (14%)	6 (1%)	15 59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	283	ARG
1	D	198	SER
1	A	198	SER
1	C	196	LEU
1	A	153	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	94/123 (76%)	84 (89%)	10 (11%)	8 36
1	B	92/123 (75%)	81 (88%)	11 (12%)	6 31
1	C	88/123 (72%)	81 (92%)	7 (8%)	15 51
1	D	88/123 (72%)	76 (86%)	12 (14%)	5 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	362/492 (74%)	322 (89%)	40 (11%)	8 35

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	TRP
1	A	161	PHE
1	A	171	LEU
1	A	197	GLU
1	A	241	MSE
1	A	258	GLN
1	A	266	GLU
1	A	267	MSE
1	A	269	GLN
1	A	281	LEU
1	B	161	PHE
1	B	171	LEU
1	B	197	GLU
1	B	198	SER
1	B	241	MSE
1	B	256	GLN
1	B	257	GLU
1	B	258	GLN
1	B	266	GLU
1	B	267	MSE
1	B	269	GLN
1	C	161	PHE
1	C	171	LEU
1	C	197	GLU
1	C	241	MSE
1	C	266	GLU
1	C	267	MSE
1	C	269	GLN
1	D	161	PHE
1	D	171	LEU
1	D	188	TYR
1	D	197	GLU
1	D	198	SER
1	D	233	PHE
1	D	236	ILE
1	D	241	MSE
1	D	266	GLU

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Mol	Chain	Res	Type
1	D	267	MSE
1	D	269	GLN
1	D	281	LEU

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

Mol	Chain	Res	Type
1	A	258	GLN
1	B	258	GLN
1	B	269	GLN

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	119/152 (78%)	-0.93	0 100 100	121, 243, 405, 464	0
1	B	108/152 (71%)	-0.90	1 (0%) 85 81	164, 301, 428, 537	0
1	C	118/152 (77%)	-0.90	0 100 100	89, 276, 435, 495	0
1	D	117/152 (76%)	-0.88	0 100 100	176, 325, 461, 538	0
All	All	462/608 (75%)	-0.90	1 (0%) 95 94	89, 291, 434, 538	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	242	GLN	3.7

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.