Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:54 AM GMT

PDB ID	:	2JAA
Title	:	SeMet substituted Shigella Flexneri Ipad
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Deposited on	:	2006-11-24
Resolution	:	3.10 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:

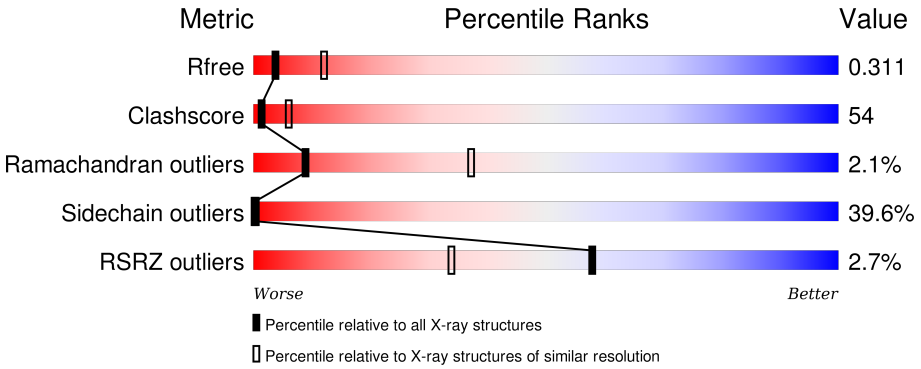
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	212	3% 20% 34% 23% • 21%
1	B	212	% 27% 40% 18% • 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2767 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 INVASIN IPAD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	Se	0	0	0
			1322	837	220	260	5			
1	B	182	Total	C	N	O	Se	0	0	0
			1437	908	239	285	5			

- Molecule 2 is water.

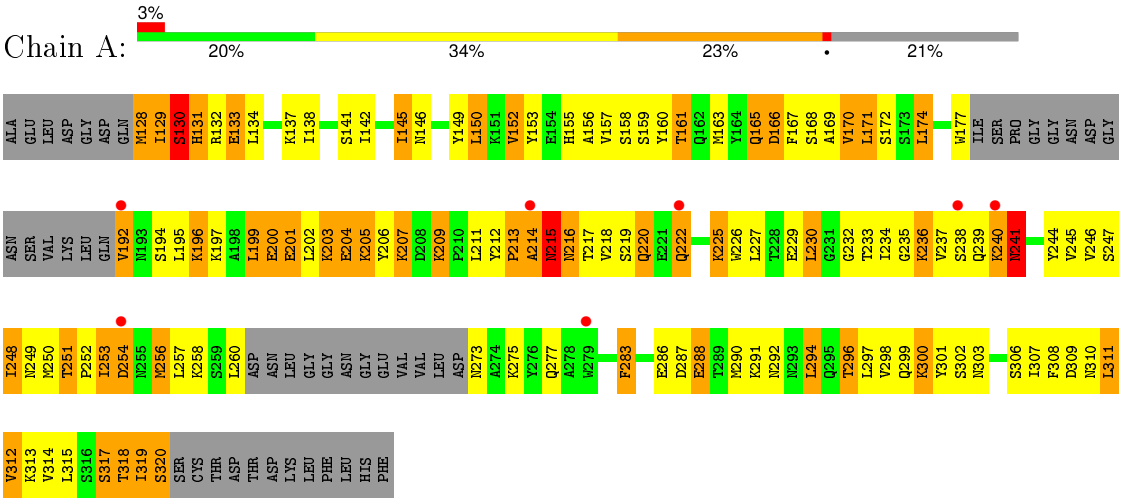
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	5	Total	O	0	0
			5	5		

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.

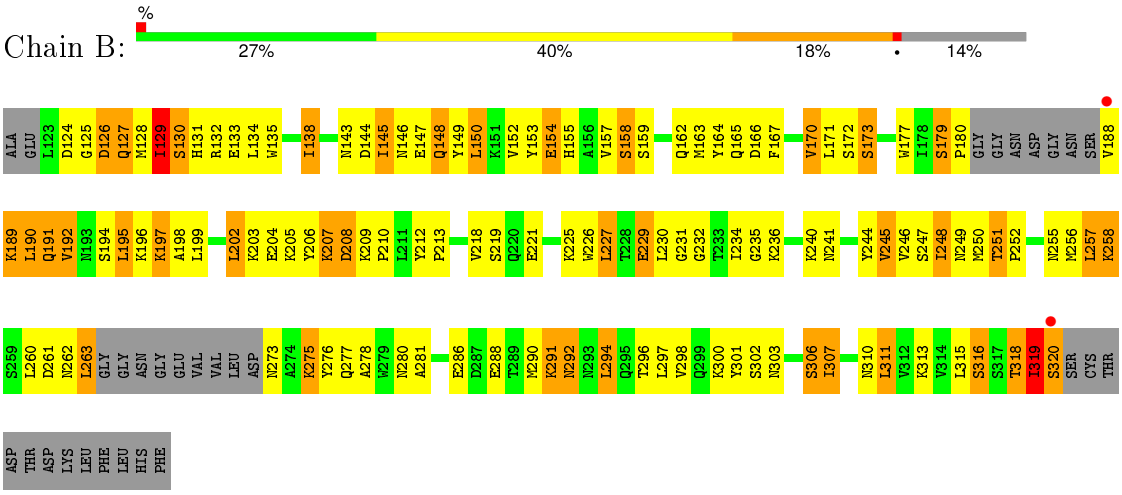
- Molecule 1: INVASIN IPAD

Chain A:



- Molecule 1: INVASIN IPAD

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	137.84Å 44.48Å 100.31Å 90.00° 107.96° 90.00°	Depositor
Resolution (Å)	34.00 – 3.10 33.92 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (34.00-3.10) 99.5 (33.92-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 3.12Å)	Xtriage
Refinement program	TNT 5.6.1	Depositor
R, R_{free}	0.262 , 0.276 0.290 , 0.311	Depositor DCC
R_{free} test set	543 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	74.4	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 83.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 10760 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	2767	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.49% 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	0.25	0/1340	0.43	1/1803 (0.1%)
1	B	0.22	0/1455	0.39	0/1958
All	All	0.23	0/2795	0.41	1/3761 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	215	ASN	N-CA-C	-7.00	92.11	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	PRO	Peptide
1	A	214	ALA	Peptide

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	1322	0	1310	179	0
1	B	1437	0	1425	133	0
2	A	3	0	0	1	0
2	B	5	0	0	0	0
All	All	2767	0	2735	294	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 54.

All (294) 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:B:195:LEU:HD13	1:B:260:LEU:HD21	1.32	1.07
1:A:318:THR:HG22	1:A:319:ILE:HG13	1.35	1.07
1:A:319:ILE:HG22	1:A:320:SER:HB2	1.47	0.95
1:A:219:SER:HB2	1:A:222:GLN:HB2	1.50	0.94
1:A:163:MSE:HA	1:A:206:TYR:CE2	2.03	0.94
1:A:206:TYR:HA	1:A:209:LYS:HG3	1.50	0.94
1:A:129:ILE:HG23	1:B:129:ILE:HD13	1.50	0.92
1:A:153:TYR:HB3	1:A:301:TYR:HD2	1.39	0.87
1:B:190:LEU:HD21	1:B:192:VAL:HG12	1.59	0.85
1:B:124:ASP:N	1:B:125:GLY:HA2	1.91	0.84
1:B:190:LEU:CD2	1:B:192:VAL:HG12	2.07	0.84
1:B:294:LEU:HD22	1:B:298:VAL:HG23	1.61	0.83
1:A:220:GLN:HG3	1:A:244:TYR:CD2	2.13	0.83
1:A:153:TYR:HB3	1:A:301:TYR:CD2	2.15	0.82
1:A:129:ILE:HG23	1:B:129:ILE:CD1	2.10	0.81
1:A:203:LYS:HG3	1:A:253:ILE:HG21	1.61	0.80
1:A:311:LEU:HD11	1:B:310:ASN:CB	2.11	0.80
1:B:177:TRP:HB3	1:B:191:GLN:HG2	1.63	0.80
1:A:152:VAL:HG11	1:A:226:TRP:CZ2	2.18	0.79
1:B:251:THR:HG22	1:B:252:PRO:HD3	1.63	0.78
1:B:236:LYS:HD3	1:B:249:ASN:HA	1.64	0.78
1:A:146:ASN:HA	1:A:150:LEU:HB2	1.67	0.77
1:A:227:LEU:CD2	1:A:232:GLY:HA2	2.15	0.76
1:A:174:LEU:HD12	1:A:195:LEU:CD1	2.15	0.76
1:B:177:TRP:HB3	1:B:191:GLN:CG	2.16	0.76
1:A:131:HIS:HB2	1:B:128:MSE:H	1.51	0.76
1:A:174:LEU:HA	1:A:177:TRP:CE3	2.21	0.75
1:B:256:MSE:O	1:B:260:LEU:HB2	1.87	0.74
1:A:227:LEU:HD23	1:A:232:GLY:HA2	1.69	0.74
1:A:318:THR:HG22	1:A:319:ILE:CG1	2.14	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:MSE:HE1	1:A:290:MSE:HE2	1.69	0.73
1:A:309:ASP:O	1:A:313:LYS:HG3	1.87	0.73
1:B:315:LEU:O	1:B:318:THR:HG22	1.89	0.72
1:A:159:SER:HB2	1:A:211:LEU:HD23	1.72	0.72
1:B:196:LYS:HB3	1:B:260:LEU:HD23	1.70	0.71
1:A:311:LEU:HD11	1:B:310:ASN:HB2	1.71	0.71
1:A:319:ILE:HG22	1:A:320:SER:CB	2.20	0.71
1:B:292:ASN:O	1:B:296:THR:HG23	1.90	0.71
1:B:195:LEU:HD13	1:B:260:LEU:CD2	2.14	0.71
1:A:195:LEU:HD22	1:A:260:LEU:HD21	1.73	0.71
1:B:227:LEU:HD22	1:B:232:GLY:HA2	1.74	0.70
1:B:129:ILE:HD12	1:B:129:ILE:H	1.56	0.69
1:B:126:ASP:HA	1:B:127:GLN:NE2	2.07	0.69
1:A:310:ASN:O	1:A:314:VAL:HG23	1.93	0.69
1:A:256:MSE:HE2	1:A:283:PHE:HD2	1.58	0.69
1:A:192:VAL:O	1:A:196:LYS:HB3	1.93	0.68
1:A:129:ILE:CG2	1:B:129:ILE:HD13	2.22	0.68
1:A:310:ASN:HB2	1:B:307:ILE:HD12	1.74	0.68
1:A:128:MSE:HA	1:B:130:SER:HA	1.75	0.68
1:A:307:ILE:HD13	1:B:306:SER:HB2	1.75	0.68
1:A:149:TYR:CE1	1:A:153:TYR:HE2	2.11	0.68
1:A:236:LYS:HD3	1:A:249:ASN:HA	1.76	0.68
1:B:213:PRO:HG3	1:B:218:VAL:HG13	1.74	0.67
1:B:205:LYS:HD3	1:B:206:TYR:CE2	2.30	0.67
1:B:227:LEU:HD21	1:B:235:GLY:O	1.95	0.67
1:B:164:TYR:OH	1:B:291:LYS:HD2	1.95	0.66
1:A:252:PRO:HG2	1:A:290:MSE:HE3	1.77	0.66
1:B:129:ILE:O	1:B:130:SER:HB2	1.95	0.66
1:A:227:LEU:HD12	1:A:237:VAL:HG12	1.78	0.65
1:A:174:LEU:HD12	1:A:195:LEU:HD11	1.78	0.65
1:A:227:LEU:HD23	1:A:227:LEU:O	1.96	0.65
1:A:318:THR:CG2	1:A:319:ILE:HG13	2.20	0.65
1:A:313:LYS:NZ	2:A:2003:HOH:O	2.30	0.65
1:A:319:ILE:CG2	1:A:320:SER:HB2	2.26	0.65
1:A:202:LEU:HD11	1:A:206:TYR:HE2	1.61	0.64
1:A:163:MSE:CE	1:A:290:MSE:HE2	2.27	0.64
1:B:149:TYR:O	1:B:152:VAL:HB	1.98	0.64
1:B:199:LEU:HB2	1:B:257:LEU:HD11	1.80	0.63
1:A:166:ASP:HB3	1:A:202:LEU:HD11	1.80	0.63
1:A:157:VAL:HG22	1:A:297:LEU:HG	1.79	0.63
1:A:251:THR:N	1:A:252:PRO:HD2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PRO:HA	1:A:286:GLU:OE1	1.98	0.63
1:A:252:PRO:O	1:A:256:MSE:HG2	1.98	0.63
1:A:256:MSE:HE2	1:A:283:PHE:CD2	2.34	0.63
1:A:236:LYS:CD	1:A:249:ASN:HA	2.28	0.63
1:A:215:ASN:O	1:A:216:ASN:HB2	1.99	0.62
1:A:213:PRO:HG2	1:A:218:VAL:HG13	1.81	0.62
1:B:203:LYS:HA	1:B:250:MSE:HE3	1.80	0.62
1:A:313:LYS:O	1:A:317:SER:HB3	2.00	0.62
1:B:199:LEU:CD1	1:B:260:LEU:HD22	2.30	0.61
1:A:252:PRO:CG	1:A:290:MSE:HE3	2.30	0.61
1:A:195:LEU:CD2	1:A:260:LEU:HD21	2.30	0.61
1:B:195:LEU:CD1	1:B:260:LEU:HD21	2.21	0.61
1:A:319:ILE:HA	1:A:320:SER:CB	2.31	0.61
1:A:157:VAL:O	1:A:161:THR:HB	2.00	0.61
1:B:196:LYS:NZ	1:B:261:ASP:OD1	2.30	0.60
1:A:196:LYS:HG3	1:A:196:LYS:O	2.01	0.60
1:A:202:LEU:HD11	1:A:206:TYR:CE2	2.37	0.60
1:A:163:MSE:SE	1:A:290:MSE:HE2	2.52	0.60
1:B:129:ILE:N	1:B:129:ILE:HD12	2.16	0.60
1:B:234:ILE:HD12	1:B:234:ILE:H	1.65	0.60
1:A:203:LYS:HG3	1:A:253:ILE:CG2	2.31	0.59
1:A:236:LYS:HD3	1:A:249:ASN:OD1	2.02	0.59
1:A:257:LEU:HD12	1:A:258:LYS:N	2.17	0.59
1:A:174:LEU:HD12	1:A:195:LEU:HD12	1.84	0.59
1:A:166:ASP:HB3	1:A:202:LEU:CD1	2.32	0.59
1:A:234:ILE:N	1:A:234:ILE:HD12	2.17	0.59
1:B:152:VAL:HG11	1:B:226:TRP:CZ2	2.38	0.59
1:B:231:GLY:HA3	1:B:234:ILE:CD1	2.33	0.59
1:A:300:LYS:NZ	1:A:300:LYS:HB2	2.17	0.59
1:A:236:LYS:HG2	1:A:249:ASN:HA	1.84	0.59
1:B:218:VAL:O	1:B:244:TYR:HB2	2.03	0.58
1:B:234:ILE:HD12	1:B:234:ILE:N	2.18	0.58
1:B:129:ILE:HG22	1:B:133:GLU:HB3	1.86	0.57
1:A:239:GLN:H	1:A:239:GLN:CD	2.08	0.57
1:B:177:TRP:O	1:B:190:LEU:HA	2.05	0.57
1:A:310:ASN:HB2	1:B:307:ILE:CD1	2.34	0.57
1:B:277:GLN:O	1:B:281:ALA:HB2	2.04	0.57
1:A:203:LYS:O	1:A:207:LYS:HB3	2.05	0.56
1:A:196:LYS:HA	1:A:260:LEU:HD23	1.87	0.56
1:A:233:THR:HG23	1:A:234:ILE:HD12	1.86	0.56
1:A:318:THR:C	1:A:319:ILE:HG13	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:MSE:HA	1:A:206:TYR:CD2	2.40	0.56
1:A:196:LYS:HE2	1:A:260:LEU:O	2.05	0.56
1:A:254:ASP:HA	1:A:257:LEU:CD2	2.36	0.56
1:B:179:SER:O	1:B:189:LYS:N	2.37	0.56
1:B:127:GLN:O	1:B:128:MSE:HB2	2.05	0.56
1:A:218:VAL:HG23	1:A:244:TYR:O	2.06	0.56
1:A:303:ASN:O	1:A:307:ILE:HG13	2.05	0.55
1:B:213:PRO:HD2	1:B:245:VAL:HB	1.88	0.55
1:B:154:GLU:HG3	1:B:155:HIS:N	2.20	0.55
1:A:288:GLU:HA	1:A:288:GLU:OE1	2.06	0.55
1:B:199:LEU:HD12	1:B:260:LEU:HD22	1.89	0.55
1:A:253:ILE:HA	1:A:256:MSE:HG3	1.88	0.55
1:A:149:TYR:CZ	1:A:153:TYR:HE2	2.25	0.54
1:A:153:TYR:CE1	1:A:300:LYS:HG3	2.43	0.54
1:A:226:TRP:CZ3	1:A:229:GLU:HG2	2.42	0.54
1:A:254:ASP:HA	1:A:257:LEU:HD21	1.89	0.54
1:A:254:ASP:O	1:A:257:LEU:HG	2.08	0.54
1:A:132:ARG:NH1	1:B:126:ASP:HB2	2.23	0.53
1:A:156:ALA:HA	1:A:211:LEU:HD22	1.89	0.53
1:A:163:MSE:CE	1:A:248:ILE:HD11	2.38	0.53
1:A:219:SER:CB	1:A:222:GLN:HB2	2.33	0.53
1:A:152:VAL:HG11	1:A:226:TRP:CE2	2.44	0.52
1:A:236:LYS:CG	1:A:249:ASN:HA	2.40	0.52
1:B:263:LEU:HG	1:B:275:LYS:NZ	2.25	0.52
1:A:145:ILE:HG21	1:A:308:PHE:CD1	2.44	0.52
1:B:212:TYR:O	1:B:246:VAL:N	2.39	0.52
1:B:206:TYR:HA	1:B:209:LYS:HG3	1.92	0.52
1:A:195:LEU:HD23	1:A:195:LEU:C	2.30	0.51
1:B:199:LEU:HD13	1:B:257:LEU:HD13	1.92	0.51
1:A:311:LEU:HD11	1:B:310:ASN:HB3	1.88	0.51
1:B:221:GLU:O	1:B:225:LYS:HG2	2.10	0.51
1:B:231:GLY:HA3	1:B:234:ILE:HD11	1.93	0.51
1:B:195:LEU:O	1:B:198:ALA:HB3	2.11	0.51
1:A:167:PHE:HA	1:A:170:VAL:HG23	1.91	0.51
1:A:142:ILE:HG12	1:A:312:VAL:HG23	1.91	0.51
1:A:196:LYS:HB2	1:A:260:LEU:HD23	1.91	0.51
1:B:235:GLY:HA2	1:B:249:ASN:H	1.75	0.51
1:A:170:VAL:HG11	1:A:199:LEU:HD23	1.93	0.51
1:A:248:ILE:HD13	1:A:248:ILE:O	2.11	0.51
1:A:213:PRO:CG	1:A:218:VAL:HG13	2.40	0.51
1:A:174:LEU:HG	1:A:174:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:VAL:O	1:B:188:VAL:HG12	2.11	0.50
1:A:196:LYS:HE2	1:A:260:LEU:HB3	1.93	0.50
1:B:248:ILE:CD1	1:B:250:MSE:SE	3.10	0.50
1:B:179:SER:O	1:B:188:VAL:HA	2.12	0.50
1:A:152:VAL:HG22	1:A:212:TYR:CD2	2.46	0.50
1:B:177:TRP:HB3	1:B:191:GLN:HG3	1.92	0.50
1:A:310:ASN:CB	1:B:307:ILE:HD12	2.40	0.50
1:B:150:LEU:O	1:B:154:GLU:HB3	2.12	0.50
1:A:192:VAL:HG23	1:A:192:VAL:O	2.11	0.50
1:A:152:VAL:HG22	1:A:212:TYR:CE2	2.47	0.50
1:B:229:GLU:OE1	1:B:229:GLU:HA	2.11	0.50
1:A:160:TYR:HD2	1:A:294:LEU:HD23	1.76	0.50
1:B:288:GLU:HA	1:B:288:GLU:OE1	2.11	0.50
1:B:152:VAL:HG11	1:B:226:TRP:CE2	2.47	0.49
1:A:246:VAL:HG12	1:A:246:VAL:O	2.11	0.49
1:A:220:GLN:HG3	1:A:244:TYR:HD2	1.72	0.49
1:A:226:TRP:O	1:A:230:LEU:HD22	2.12	0.49
1:B:138:ILE:HB	1:B:315:LEU:HD13	1.94	0.49
1:B:192:VAL:O	1:B:196:LYS:HG2	2.12	0.49
1:A:245:VAL:HG23	1:A:246:VAL:N	2.26	0.49
1:A:239:GLN:HB3	1:A:244:TYR:CE1	2.46	0.49
1:B:251:THR:O	1:B:255:ASN:OD1	2.31	0.49
1:A:309:ASP:O	1:A:312:VAL:HG12	2.13	0.49
1:A:233:THR:CG2	1:A:234:ILE:HD12	2.43	0.49
1:A:166:ASP:O	1:A:169:ALA:HB3	2.13	0.48
1:A:205:LYS:HE3	1:A:206:TYR:CZ	2.48	0.48
1:B:230:LEU:O	1:B:234:ILE:HD13	2.13	0.48
1:A:220:GLN:CD	1:A:220:GLN:H	2.16	0.48
1:A:134:LEU:O	1:A:137:LYS:HB2	2.13	0.48
1:B:197:LYS:HD2	1:B:197:LYS:HA	1.48	0.48
1:B:192:VAL:O	1:B:196:LYS:HE2	2.13	0.48
1:A:250:MSE:C	1:A:252:PRO:HD2	2.34	0.48
1:A:251:THR:N	1:A:252:PRO:CD	2.77	0.48
1:A:257:LEU:C	1:A:257:LEU:HD12	2.33	0.48
1:A:195:LEU:HD23	1:A:199:LEU:HG	1.95	0.48
1:B:255:ASN:ND2	1:B:286:GLU:OE2	2.47	0.48
1:A:130:SER:OG	1:A:133:GLU:HB2	2.13	0.47
1:A:253:ILE:HD13	1:A:290:MSE:HE1	1.96	0.47
1:A:152:VAL:HG12	1:A:153:TYR:N	2.29	0.47
1:A:292:ASN:O	1:A:296:THR:HG23	2.14	0.47
1:A:129:ILE:CG1	1:A:130:SER:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASN:O	1:B:147:GLU:HG2	2.14	0.47
1:B:170:VAL:HA	1:B:173:SER:OG	2.15	0.47
1:A:294:LEU:O	1:A:298:VAL:HG23	2.15	0.47
1:A:153:TYR:CB	1:A:301:TYR:HD2	2.20	0.47
1:B:226:TRP:O	1:B:230:LEU:HG	2.14	0.47
1:B:319:ILE:HA	1:B:320:SER:HA	1.73	0.47
1:B:303:ASN:O	1:B:307:ILE:HG12	2.15	0.47
1:A:277:GLN:OE1	1:A:277:GLN:HA	2.14	0.47
1:B:196:LYS:C	1:B:198:ALA:H	2.18	0.47
1:B:244:TYR:C	1:B:245:VAL:HG12	2.35	0.47
1:B:199:LEU:HD12	1:B:260:LEU:CD2	2.45	0.46
1:A:235:GLY:HA2	1:A:249:ASN:H	1.81	0.46
1:B:258:LYS:O	1:B:262:ASN:OD1	2.33	0.46
1:A:174:LEU:HA	1:A:177:TRP:CD2	2.49	0.46
1:B:263:LEU:HG	1:B:275:LYS:HZ1	1.80	0.46
1:B:144:ASP:O	1:B:148:GLN:HB2	2.14	0.46
1:A:253:ILE:CD1	1:A:290:MSE:HE1	2.46	0.45
1:B:210:PRO:HB3	1:B:245:VAL:CG2	2.46	0.45
1:B:234:ILE:O	1:B:249:ASN:HB3	2.17	0.45
1:B:318:THR:O	1:B:318:THR:HG23	2.15	0.45
1:B:286:GLU:HA	1:B:286:GLU:OE1	2.16	0.45
1:B:202:LEU:HA	1:B:202:LEU:HD23	1.76	0.45
1:A:227:LEU:CD1	1:A:237:VAL:HG12	2.44	0.45
1:B:248:ILE:HD13	1:B:248:ILE:O	2.17	0.45
1:B:294:LEU:HD22	1:B:298:VAL:CG2	2.39	0.45
1:B:129:ILE:HB	1:B:130:SER:H	1.50	0.45
1:A:300:LYS:HZ2	1:A:300:LYS:HB2	1.82	0.45
1:A:312:VAL:CG1	1:A:313:LYS:N	2.80	0.45
1:A:240:LYS:O	1:A:241:ASN:OD1	2.35	0.45
1:A:248:ILE:C	1:A:248:ILE:HD13	2.37	0.45
1:B:166:ASP:CB	1:B:202:LEU:HD21	2.47	0.45
1:A:170:VAL:O	1:A:174:LEU:HB3	2.17	0.44
1:A:307:ILE:HA	1:B:307:ILE:HD11	1.99	0.44
1:B:248:ILE:HD13	1:B:248:ILE:C	2.37	0.44
1:B:157:VAL:HG22	1:B:297:LEU:HG	1.99	0.44
1:B:173:SER:HB2	1:B:177:TRP:CZ2	2.53	0.44
1:A:199:LEU:O	1:A:203:LYS:HB2	2.17	0.44
1:A:156:ALA:HA	1:A:211:LEU:CD2	2.47	0.44
1:A:165:GLN:HA	1:A:165:GLN:OE1	2.11	0.44
1:B:135:TRP:CZ2	1:B:319:ILE:CG2	3.00	0.44
1:A:207:LYS:HB2	1:A:207:LYS:HE2	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LYS:HA	1:B:225:LYS:HD3	1.75	0.44
1:A:319:ILE:CA	1:A:320:SER:CB	2.96	0.44
1:B:166:ASP:HB3	1:B:202:LEU:HD21	2.00	0.44
1:B:205:LYS:HD3	1:B:206:TYR:HE2	1.80	0.44
1:A:145:ILE:HG21	1:A:308:PHE:HD1	1.83	0.44
1:B:316:SER:C	1:B:318:THR:H	2.21	0.43
1:B:202:LEU:HD22	1:B:206:TYR:CE2	2.53	0.43
1:A:256:MSE:CE	1:A:283:PHE:CD2	3.00	0.43
1:B:240:LYS:HB3	1:B:245:VAL:CG1	2.49	0.43
1:A:174:LEU:HD23	1:A:174:LEU:C	2.39	0.43
1:A:300:LYS:NZ	1:A:300:LYS:CB	2.79	0.43
1:B:318:THR:CG2	1:B:319:ILE:HG12	2.48	0.43
1:A:256:MSE:HE3	1:A:286:GLU:HB2	2.01	0.43
1:B:252:PRO:O	1:B:256:MSE:HG3	2.19	0.43
1:A:273:ASN:O	1:A:277:GLN:N	2.41	0.43
1:A:200:GLU:O	1:A:204:GLU:OE2	2.36	0.43
1:A:152:VAL:CG2	1:A:212:TYR:CE2	3.01	0.43
1:B:278:ALA:O	1:B:281:ALA:HB3	2.19	0.42
1:B:171:LEU:HA	1:B:171:LEU:HD23	1.90	0.42
1:A:219:SER:HB2	1:A:222:GLN:CB	2.36	0.42
1:A:234:ILE:N	1:A:234:ILE:CD1	2.80	0.42
1:B:166:ASP:OD2	1:B:205:LYS:HE2	2.19	0.42
1:A:171:LEU:HD23	1:A:172:SER:N	2.35	0.42
1:A:177:TRP:CZ3	1:A:195:LEU:HA	2.55	0.42
1:B:145:ILE:O	1:B:149:TYR:N	2.47	0.42
1:A:201:GLU:OE1	1:A:201:GLU:HA	2.19	0.42
1:A:319:ILE:CA	1:A:320:SER:HB2	2.50	0.42
1:B:179:SER:HA	1:B:180:PRO:HD3	1.77	0.42
1:A:225:LYS:HG2	1:A:225:LYS:H	1.44	0.42
1:A:130:SER:O	1:A:131:HIS:HB2	2.20	0.42
1:B:124:ASP:N	1:B:125:GLY:CA	2.73	0.42
1:B:318:THR:HG22	1:B:319:ILE:CG1	2.50	0.42
1:A:149:TYR:CE1	1:A:153:TYR:CE2	3.01	0.41
1:B:263:LEU:HD23	1:B:263:LEU:HA	1.75	0.41
1:A:153:TYR:HE1	1:A:300:LYS:HG3	1.84	0.41
1:A:314:VAL:HG11	1:B:311:LEU:HD11	2.02	0.41
1:A:174:LEU:CD1	1:A:195:LEU:HD11	2.49	0.41
1:A:196:LYS:CA	1:A:260:LEU:HD23	2.50	0.41
1:A:163:MSE:HE1	1:A:290:MSE:CE	2.45	0.41
1:B:230:LEU:C	1:B:234:ILE:HD13	2.40	0.41
1:A:307:ILE:HD13	1:B:306:SER:CB	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:TYR:HB2	1:B:250:MSE:HE2	2.02	0.41
1:B:167:PHE:O	1:B:170:VAL:HG12	2.20	0.41
1:A:163:MSE:HG2	1:A:206:TYR:CD2	2.55	0.41
1:B:191:GLN:HG2	1:B:191:GLN:H	1.42	0.41
1:A:174:LEU:CA	1:A:177:TRP:CE3	3.00	0.41
1:B:127:GLN:N	1:B:127:GLN:CD	2.73	0.41
1:A:156:ALA:CA	1:A:211:LEU:HD22	2.48	0.41
1:B:207:LYS:HD2	1:B:208:ASP:OD2	2.20	0.41
1:A:155:HIS:CD2	1:A:214:ALA:HB2	2.55	0.41
1:A:145:ILE:CG2	1:A:308:PHE:CD1	3.04	0.41
1:B:158:SER:O	1:B:162:GLN:HG3	2.21	0.41
1:B:167:PHE:CE1	1:B:290:MSE:HE1	2.56	0.40
1:A:132:ARG:HG3	1:B:126:ASP:OD1	2.22	0.40
1:A:236:LYS:HD3	1:A:249:ASN:CG	2.40	0.40
1:B:163:MSE:HE2	1:B:248:ILE:HD11	2.03	0.40
1:A:142:ILE:CD1	1:A:312:VAL:CG2	3.00	0.40
1:A:132:ARG:HG3	1:B:126:ASP:CG	2.41	0.40
1:B:153:TYR:HB3	1:B:301:TYR:CD2	2.57	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	161/212 (76%)	141 (88%)	16 (10%)	4 (2%)	7 32
1	B	176/212 (83%)	154 (88%)	19 (11%)	3 (2%)	11 43
All	All	337/424 (80%)	295 (88%)	35 (10%)	7 (2%)	9 37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	A	216	ASN
1	B	130	SER
1	B	319	ILE
1	A	130	SER
1	A	241	ASN
1	B	129	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	147/179 (82%)	83 (56%)	64 (44%)	0 0
1	B	161/179 (90%)	103 (64%)	58 (36%)	0 0
All	All	308/358 (86%)	186 (60%)	122 (40%)	0 0

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	MSE
1	A	129	ILE
1	A	130	SER
1	A	131	HIS
1	A	133	GLU
1	A	138	ILE
1	A	141	SER
1	A	145	ILE
1	A	150	LEU
1	A	152	VAL
1	A	158	SER
1	A	161	THR
1	A	165	GLN
1	A	166	ASP
1	A	168	SER
1	A	170	VAL
1	A	171	LEU

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Mol	Chain	Res	Type
1	A	174	LEU
1	A	192	VAL
1	A	194	SER
1	A	196	LYS
1	A	197	LYS
1	A	199	LEU
1	A	200	GLU
1	A	201	GLU
1	A	203	LYS
1	A	204	GLU
1	A	205	LYS
1	A	207	LYS
1	A	209	LYS
1	A	215	ASN
1	A	217	THR
1	A	220	GLN
1	A	222	GLN
1	A	225	LYS
1	A	230	LEU
1	A	236	LYS
1	A	238	SER
1	A	240	LYS
1	A	241	ASN
1	A	247	SER
1	A	248	ILE
1	A	251	THR
1	A	253	ILE
1	A	254	ASP
1	A	256	MSE
1	A	275	LYS
1	A	283	PHE
1	A	287	ASP
1	A	288	GLU
1	A	291	LYS
1	A	294	LEU
1	A	296	THR
1	A	299	GLN
1	A	300	LYS
1	A	302	SER
1	A	306	SER
1	A	311	LEU
1	A	312	VAL

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Mol	Chain	Res	Type
1	A	315	LEU
1	A	317	SER
1	A	318	THR
1	A	319	ILE
1	A	320	SER
1	B	126	ASP
1	B	127	GLN
1	B	129	ILE
1	B	131	HIS
1	B	132	ARG
1	B	134	LEU
1	B	138	ILE
1	B	145	ILE
1	B	146	ASN
1	B	148	GLN
1	B	150	LEU
1	B	154	GLU
1	B	158	SER
1	B	159	SER
1	B	165	GLN
1	B	170	VAL
1	B	172	SER
1	B	173	SER
1	B	179	SER
1	B	189	LYS
1	B	190	LEU
1	B	191	GLN
1	B	192	VAL
1	B	194	SER
1	B	195	LEU
1	B	197	LYS
1	B	202	LEU
1	B	204	GLU
1	B	207	LYS
1	B	208	ASP
1	B	219	SER
1	B	227	LEU
1	B	229	GLU
1	B	241	ASN
1	B	245	VAL
1	B	247	SER
1	B	248	ILE

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Mol	Chain	Res	Type
1	B	251	THR
1	B	257	LEU
1	B	258	LYS
1	B	263	LEU
1	B	273	ASN
1	B	275	LYS
1	B	276	TYR
1	B	280	ASN
1	B	291	LYS
1	B	292	ASN
1	B	294	LEU
1	B	300	LYS
1	B	302	SER
1	B	306	SER
1	B	307	ILE
1	B	311	LEU
1	B	313	LYS
1	B	316	SER
1	B	318	THR
1	B	319	ILE
1	B	320	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	215	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 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	162/212 (76%)	0.27	7 (4%)	39	18	35, 80, 108, 118	0
1	B	177/212 (83%)	0.01	2 (1%)	82	66	28, 65, 101, 130	0
All	All	339/424 (79%)	0.14	9 (2%)	58	34	28, 69, 105, 130	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	SER	4.7
1	B	188	VAL	3.1
1	A	214	ALA	2.7
1	A	192	VAL	2.6
1	A	240	LYS	2.6
1	B	320	SER	2.3
1	A	254	ASP	2.1
1	A	222	GLN	2.0
1	A	279	TRP	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.