Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:35 PM GMT

PDB ID	:	4LVN
Title	:	Crystal structure of PfSUB1-prodomain-NIMP.M7 Fab complex
Authors	:	Withers-Martinez, C.; Blackman, M.J.
Deposited on	:	2013-07-26
Resolution	:	2.25 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 ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

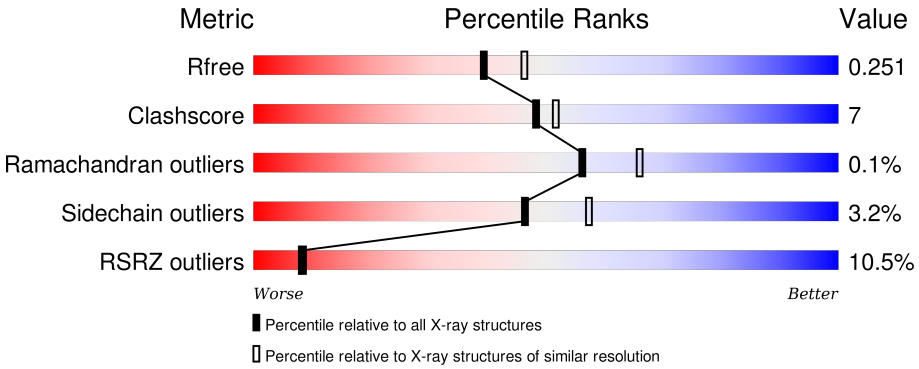
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	344	8% 80% 17%
2	B	212	8% 79% 16%
3	C	220	9% 82% 15%
4	P	93	24% 71% 15% 13%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6622 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 Subtilisin-like serine protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	1	0
			2632	1656	455	507	14			

- Molecule 2 is a protein called NIMP.M7 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	S	0	0	0
			1524	947	257	312	8			

- Molecule 3 is a protein called NIMP.M7 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	216	Total	C	N	O	S	0	0	0
			1608	1026	258	318	6			

- Molecule 4 is a protein called Subtilisin-like serine protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	81	Total	C	N	O	S	0	0	0
			639	404	99	135	1			

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	Ni	0	0
			1	1		
5	A	1	Total	Ni	0	0
			1	1		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Ca 3 3	0	0

- Molecule 7 is water.

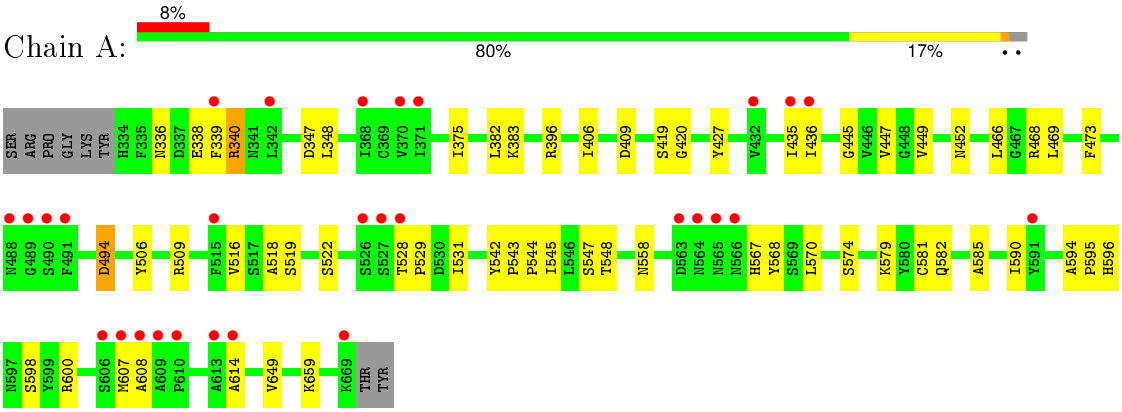
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	92	Total O 92 92	0	0
7	B	67	Total O 67 67	0	0
7	C	49	Total O 49 49	0	0
7	P	6	Total O 6 6	0	0

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.

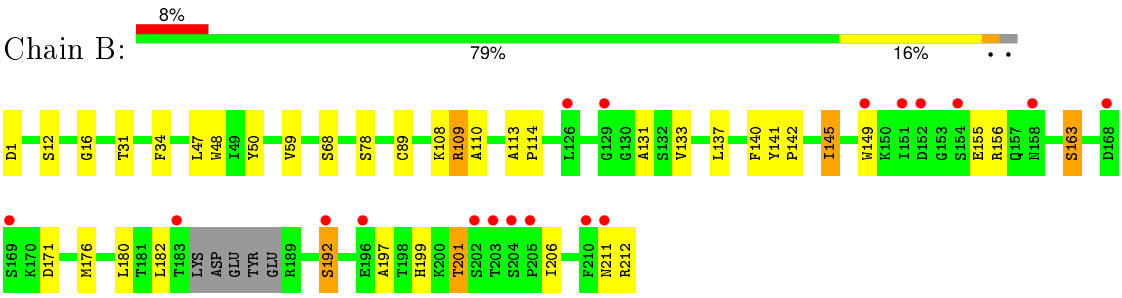
- Molecule 1: Subtilisin-like serine protease

Chain A:



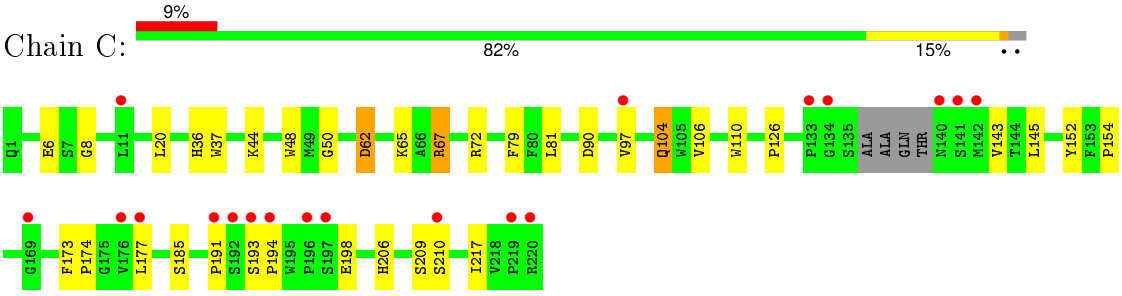
- Molecule 2: NIMP.M7 Fab light chain

Chain B:



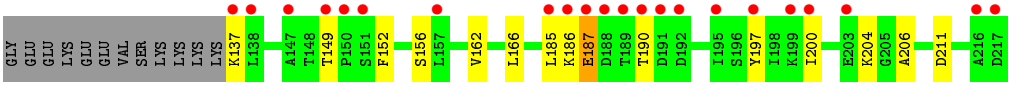
- Molecule 3: NIMP.M7 Fab heavy chain

Chain C:



- Molecule 4: Subtilisin-like serine protease

Chain P:


GLY
GLU
GLU
LYS
GLU
GLU
VAL
SER
LYS
LYS
LYS
LYS
K137
L138
A147
T148
T149
P150
S151
F152
S156
L157
V162
L166
L185
K186
E187
D188
T189
T190
D191
D192
I195
S196
Y197
I198
K199
I200
E203
K204
G205
A206
D211
A216
D217

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.50Å 74.79Å 78.85Å 90.00° 103.33° 90.00°	Depositor
Resolution (Å)	29.88 – 2.25 29.88 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.88-2.25) 98.2 (29.88-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.195 , 0.237 0.204 , 0.251	Depositor DCC
R_{free} test set	1953 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 38909 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6622	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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: NI, CA

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	0.27	0/2689	0.47	0/3642
2	B	0.27	0/1562	0.45	0/2131
3	C	0.27	0/1656	0.50	0/2279
4	P	0.25	0/645	0.47	0/868
All	All	0.27	0/6552	0.47	0/8920

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2632	0	2570	36	0
2	B	1524	0	1398	27	0
3	C	1608	0	1501	22	0
4	P	639	0	648	10	0
5	A	1	0	0	0	0
5	P	1	0	0	0	0
6	A	3	0	0	0	0
7	A	92	0	0	4	0
7	B	67	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	49	0	0	0	0
7	P	6	0	0	0	0
All	All	6622	0	6117	91	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 7.

All (91) 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)
3:C:62:ASP:HA	3:C:65:LYS:HG2	1.70	0.72
3:C:206:HIS:ND1	3:C:209:SER:OG	2.26	0.69
2:B:145:ILE:HD12	2:B:199:HIS:HB2	1.76	0.67
3:C:145:LEU:HD22	3:C:217:ILE:HG21	1.76	0.67
2:B:156:ARG:HH12	2:B:182:LEU:HB3	1.61	0.64
1:A:558:ASN:HB3	1:A:574:SER:HB2	1.82	0.62
2:B:137:LEU:HD13	2:B:176:MET:HE3	1.81	0.61
1:A:468:ARG:HD3	4:P:137:LYS:HE2	1.83	0.60
1:A:494:ASP:OD1	1:A:494:ASP:N	2.35	0.60
1:A:581[B]:CYS:HB3	1:A:649:VAL:HG12	1.83	0.59
3:C:36:HIS:HB2	3:C:97:VAL:HG12	1.84	0.59
2:B:149:TRP:O	2:B:155:GLU:HA	2.02	0.58
1:A:419:SER:HB2	1:A:420:GLY:HA3	1.85	0.58
2:B:34:PHE:CZ	2:B:89:CYS:HB2	2.40	0.57
1:A:547:SER:HB2	1:A:582:GLN:HE22	1.69	0.57
2:B:163:SER:HB3	3:C:173:PHE:HB3	1.87	0.56
1:A:435:ILE:HD11	1:A:607:MET:HG3	1.89	0.54
1:A:339:PHE:N	7:A:875:HOH:O	2.38	0.54
2:B:12:SER:HB3	2:B:108:LYS:HG3	1.91	0.53
1:A:436:ILE:HG23	1:A:614:ALA:HB2	1.92	0.52
1:A:340:ARG:HH22	1:A:347:ASP:N	2.08	0.52
2:B:131:ALA:HB3	2:B:182:LEU:HD12	1.91	0.52
2:B:109:ARG:HH21	2:B:171:ASP:HB2	1.75	0.51
2:B:133:VAL:HG13	2:B:180:LEU:HB3	1.92	0.51
2:B:156:ARG:NH1	2:B:182:LEU:HB3	2.25	0.51
3:C:194:PRO:O	3:C:198:GLU:N	2.36	0.51
3:C:72:ARG:HA	3:C:79:PHE:HA	1.91	0.50
3:C:126:PRO:HB3	3:C:152:TYR:HB3	1.94	0.50
2:B:156:ARG:HD3	2:B:180:LEU:HD11	1.94	0.49
3:C:104:GLN:HG2	3:C:106:VAL:H	1.77	0.49
1:A:594:ALA:HB2	1:A:600:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:HG	1:A:473:PHE:HE1	1.79	0.47
2:B:47:LEU:HD21	2:B:50:TYR:HB3	1.96	0.47
3:C:104:GLN:CG	3:C:106:VAL:HG12	2.44	0.47
4:P:200:ILE:O	4:P:204:LYS:HG2	2.15	0.47
4:P:186:LYS:HB2	4:P:186:LYS:HE3	1.56	0.47
3:C:209:SER:N	3:C:210:SER:HA	2.29	0.47
1:A:506:TYR:HA	1:A:509:ARG:HG2	1.97	0.47
1:A:548:THR:HG21	1:A:579:LYS:HG2	1.97	0.47
4:P:186:LYS:HA	4:P:187:GLU:HA	1.55	0.46
1:A:375:ILE:HD11	1:A:382:LEU:HD13	1.96	0.46
1:A:383:LYS:NZ	7:A:819:HOH:O	2.48	0.46
4:P:166:LEU:HA	4:P:197:TYR:HE1	1.80	0.46
2:B:199:HIS:ND1	2:B:201:THR:OG1	2.43	0.46
2:B:156:ARG:HH11	2:B:180:LEU:HD11	1.81	0.46
2:B:1:ASP:OD1	2:B:1:ASP:N	2.42	0.46
1:A:659:LYS:HA	1:A:659:LYS:HD2	1.80	0.45
1:A:449:VAL:HB	1:A:614:ALA:HB3	1.99	0.45
4:P:152:PHE:HA	4:P:156:SER:HB2	1.99	0.45
3:C:191:PRO:HB2	3:C:194:PRO:HD2	1.98	0.44
1:A:516:VAL:HG11	1:A:543:PRO:HG2	1.99	0.44
2:B:31:THR:HG22	2:B:68:SER:HA	2.00	0.44
1:A:336:ASN:HB3	1:A:338:GLU:OE1	2.17	0.44
2:B:206:ILE:HA	2:B:206:ILE:HD12	1.89	0.44
1:A:468:ARG:HB3	4:P:211:ASP:OD2	2.18	0.44
3:C:44:LYS:HD2	3:C:44:LYS:HA	1.85	0.44
4:P:152:PHE:CG	4:P:206:ALA:HB2	2.54	0.43
3:C:67:ARG:NH2	3:C:90:ASP:OD1	2.42	0.43
4:P:185:LEU:HD21	4:P:197:TYR:CE2	2.53	0.43
2:B:192:SER:HA	2:B:211:ASN:OD1	2.19	0.43
2:B:48:TRP:O	2:B:59:VAL:HG21	2.18	0.43
1:A:518:ALA:O	1:A:519:SER:HB3	2.19	0.43
1:A:547:SER:HB2	1:A:582:GLN:NE2	2.33	0.43
2:B:163:SER:OG	3:C:174:PRO:O	2.33	0.43
1:A:348:LEU:HD13	1:A:568:TYR:CZ	2.53	0.42
1:A:466:LEU:HD23	1:A:466:LEU:HA	1.86	0.42
2:B:141:TYR:CG	2:B:142:PRO:HA	2.54	0.42
2:B:109:ARG:HG2	2:B:110:ALA:N	2.34	0.42
3:C:37:TRP:CE2	3:C:81:LEU:HB2	2.54	0.42
1:A:406:ILE:HG21	1:A:409:ASP:HB3	2.02	0.42
2:B:113:ALA:N	2:B:201:THR:HG21	2.35	0.41
1:A:585:ALA:HB3	1:A:608:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:TYR:C	1:A:544:PRO:HD2	2.40	0.41
2:B:197:ALA:HB3	2:B:206:ILE:HG22	2.02	0.41
1:A:528:THR:HA	1:A:529:PRO:HD3	1.91	0.41
1:A:596:HIS:NE2	7:A:873:HOH:O	2.25	0.41
2:B:16:GLY:HA2	2:B:78:SER:OG	2.20	0.41
3:C:8:GLY:HA3	3:C:20:LEU:HD23	2.02	0.41
1:A:396:ARG:HD2	7:A:892:HOH:O	2.21	0.41
3:C:177:LEU:HA	3:C:177:LEU:HD23	1.93	0.41
3:C:48:TRP:CZ2	3:C:50:GLY:HA2	2.56	0.41
3:C:97:VAL:HG23	3:C:110:TRP:HA	2.03	0.41
4:P:162:VAL:HG21	4:P:204:LYS:HE2	2.03	0.41
2:B:114:PRO:CA	2:B:140:PHE:HB3	2.51	0.41
1:A:543:PRO:N	1:A:544:PRO:HD2	2.35	0.40
1:A:595:PRO:O	1:A:598:SER:HB3	2.21	0.40
1:A:590:ILE:HG13	1:A:607:MET:HB3	2.04	0.40
1:A:339:PHE:CE1	1:A:445:GLY:HA2	2.57	0.40
1:A:570:LEU:HA	1:A:570:LEU:HD12	1.87	0.40
3:C:154:PRO:O	3:C:206:HIS:NE2	2.43	0.40
3:C:6:GLU:OE1	3:C:6:GLU:N	2.54	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	335/344 (97%)	323 (96%)	11 (3%)	1 (0%)	46 52
2	B	203/212 (96%)	190 (94%)	13 (6%)	0	100 100
3	C	212/220 (96%)	202 (95%)	10 (5%)	0	100 100
4	P	79/93 (85%)	76 (96%)	3 (4%)	0	100 100
All	All	829/869 (95%)	791 (95%)	37 (4%)	1 (0%)	56 66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	427	TYR

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	297/303 (98%)	289 (97%)	8 (3%)	52	63
2	B	168/186 (90%)	162 (96%)	6 (4%)	42	51
3	C	178/194 (92%)	172 (97%)	6 (3%)	44	54
4	P	76/87 (87%)	73 (96%)	3 (4%)	39	48
All	All	719/770 (93%)	696 (97%)	23 (3%)	46	57

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	ARG
1	A	447	VAL
1	A	452	ASN
1	A	494	ASP
1	A	522	SER
1	A	531	ILE
1	A	545	ILE
1	A	567	HIS
2	B	109	ARG
2	B	145	ILE
2	B	163	SER
2	B	192	SER
2	B	201	THR
2	B	212	ARG
3	C	62	ASP
3	C	67	ARG
3	C	104	GLN
3	C	143	VAL
3	C	185	SER

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Mol	Chain	Res	Type
3	C	193	SER
4	P	149	THR
4	P	187	GLU
4	P	190	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (i)

Of 5 ligands modelled in this entry, 5 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 (i)

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	336/344 (97%)	0.54	29 (8%)	13	14	23, 39, 69, 128	1 (0%)
2	B	207/212 (97%)	0.58	18 (8%)	13	14	24, 49, 88, 108	0
3	C	216/220 (98%)	0.51	19 (8%)	12	14	25, 52, 89, 106	0
4	P	81/93 (87%)	1.45	22 (27%)	1	0	43, 73, 104, 126	0
All	All	840/869 (96%)	0.63	88 (10%)	8	8	23, 46, 90, 128	1 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	563	ASP	6.4
2	B	152	ASP	5.4
4	P	150	PRO	5.3
1	A	565	ASN	5.3
4	P	189	THR	5.1
1	A	526	SER	5.1
4	P	188	ASP	5.0
4	P	187	GLU	5.0
1	A	564	ASN	4.8
1	A	669	LYS	4.7
4	P	138	LEU	4.7
2	B	205	PRO	4.6
2	B	192	SER	4.5
2	B	151	ILE	4.5
4	P	191	ASP	4.5
1	A	339	PHE	4.3
2	B	158	ASN	4.2
4	P	186	LYS	3.9
2	B	202	SER	3.9
1	A	609	ALA	3.8
2	B	126	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	608	ALA	3.5
3	C	177	LEU	3.4
2	B	154	SER	3.4
4	P	216	ALA	3.4
2	B	169	SER	3.3
3	C	197	SER	3.3
1	A	527	SER	3.3
2	B	149	TRP	3.2
4	P	190	THR	3.2
3	C	134	GLY	3.2
3	C	191	PRO	3.2
4	P	149	THR	3.2
4	P	217	ASP	3.1
3	C	11	LEU	3.1
4	P	157	LEU	3.1
3	C	141	SER	3.0
4	P	137	LYS	3.0
1	A	607	MET	3.0
1	A	528	THR	3.0
1	A	566	ASN	2.9
1	A	610	PRO	2.9
3	C	220	ARG	2.9
4	P	192	ASP	2.9
4	P	185	LEU	2.9
2	B	129	GLY	2.9
1	A	488	ASN	2.9
1	A	490	SER	2.9
4	P	199	LYS	2.8
4	P	200	ILE	2.8
3	C	219	PRO	2.8
1	A	591	TYR	2.8
1	A	436	ILE	2.7
1	A	489	GLY	2.7
3	C	140	ASN	2.6
4	P	197	TYR	2.6
1	A	613	ALA	2.6
3	C	97	VAL	2.6
4	P	195	ILE	2.6
2	B	168	ASP	2.6
3	C	176	VAL	2.6
1	A	432	VAL	2.6
3	C	194	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
4	P	147	ALA	2.5
3	C	193	SER	2.4
1	A	515	PHE	2.4
3	C	142	MET	2.4
1	A	370	VAL	2.4
1	A	435	ILE	2.4
4	P	151	SER	2.4
2	B	210	PHE	2.3
4	P	203	GLU	2.3
1	A	342	LEU	2.2
1	A	606	SER	2.2
3	C	169	GLY	2.2
2	B	203	THR	2.2
1	A	491	PHE	2.2
3	C	196	PRO	2.2
2	B	183	THR	2.2
3	C	192	SER	2.2
3	C	210	SER	2.1
1	A	614	ALA	2.1
1	A	368	ILE	2.1
1	A	371	ILE	2.1
2	B	196	GLU	2.1
2	B	211	ASN	2.1
2	B	204	SER	2.0
3	C	133	PRO	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)

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
6	CA	A	704	1/1	1.00	0.08	-1.73	31,31,31,31	0
6	CA	A	703	1/1	0.99	0.08	-1.97	31,31,31,31	0
6	CA	A	702	1/1	0.98	0.06	-2.87	33,33,33,33	0
5	NI	P	301	1/1	0.98	0.06	-	55,55,55,55	0
5	NI	A	701	1/1	0.71	0.12	-	81,81,81,81	0

6.5 Other polymers

There are no such residues in this entry.