Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 02:34 PM EDT

PDB ID	:	3I48
Title	:	Crystal structure of beta toxin from Staphylococcus aureus F277A, P278A mutant with bound magnesium ions
Authors	:	Huseby, M.; Shi, K.; Kruse, A.C.; Ohlendorf, D.H.
Deposited on	:	2009-07-01
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

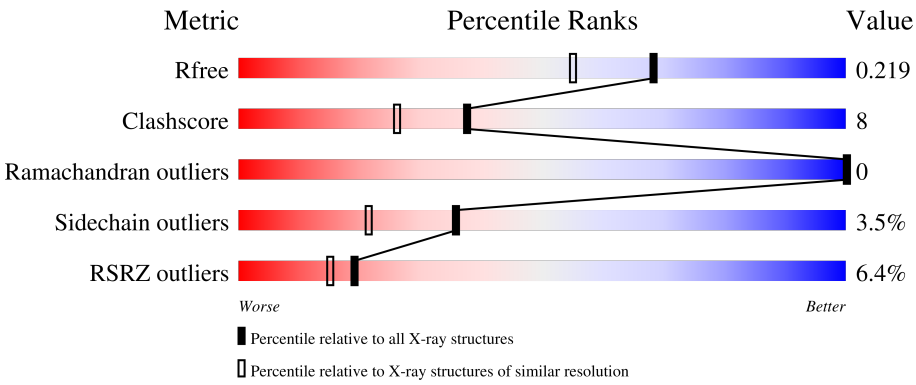
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	8%, 77%, 13%, • 8%
1	B	317	3%, 77%, 14%, 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	403	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5150 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 Beta-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	291	2337	1481	394	457	5	0	0	0
1	B	290	2329	1477	393	454	5	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A7LAI8
A	-18	ARG	-	expression tag	UNP A7LAI8
A	-17	SER	-	expression tag	UNP A7LAI8
A	-16	SER	-	expression tag	UNP A7LAI8
A	-15	HIS	-	expression tag	UNP A7LAI8
A	-14	HIS	-	expression tag	UNP A7LAI8
A	-13	HIS	-	expression tag	UNP A7LAI8
A	-12	HIS	-	expression tag	UNP A7LAI8
A	-11	HIS	-	expression tag	UNP A7LAI8
A	-10	HIS	-	expression tag	UNP A7LAI8
A	-9	SER	-	expression tag	UNP A7LAI8
A	-8	SER	-	expression tag	UNP A7LAI8
A	-7	GLY	-	expression tag	UNP A7LAI8
A	-6	LEU	-	expression tag	UNP A7LAI8
A	-5	VAL	-	expression tag	UNP A7LAI8
A	-4	PRO	-	expression tag	UNP A7LAI8
A	-3	ARG	-	expression tag	UNP A7LAI8
A	-2	GLY	-	expression tag	UNP A7LAI8
A	-1	SER	-	expression tag	UNP A7LAI8
A	0	HIS	-	expression tag	UNP A7LAI8
A	1	MET	-	expression tag	UNP A7LAI8
A	277	ALA	PHE	engineered mutation	UNP A7LAI8
A	278	ALA	PRO	engineered mutation	UNP A7LAI8
B	-19	MET	-	expression tag	UNP A7LAI8
B	-18	ARG	-	expression tag	UNP A7LAI8

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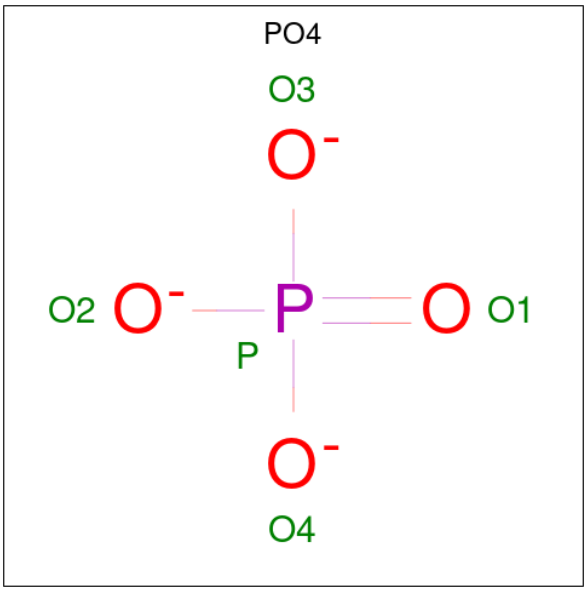
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP A7LAI8
B	-16	SER	-	expression tag	UNP A7LAI8
B	-15	HIS	-	expression tag	UNP A7LAI8
B	-14	HIS	-	expression tag	UNP A7LAI8
B	-13	HIS	-	expression tag	UNP A7LAI8
B	-12	HIS	-	expression tag	UNP A7LAI8
B	-11	HIS	-	expression tag	UNP A7LAI8
B	-10	HIS	-	expression tag	UNP A7LAI8
B	-9	SER	-	expression tag	UNP A7LAI8
B	-8	SER	-	expression tag	UNP A7LAI8
B	-7	GLY	-	expression tag	UNP A7LAI8
B	-6	LEU	-	expression tag	UNP A7LAI8
B	-5	VAL	-	expression tag	UNP A7LAI8
B	-4	PRO	-	expression tag	UNP A7LAI8
B	-3	ARG	-	expression tag	UNP A7LAI8
B	-2	GLY	-	expression tag	UNP A7LAI8
B	-1	SER	-	expression tag	UNP A7LAI8
B	0	HIS	-	expression tag	UNP A7LAI8
B	1	MET	-	expression tag	UNP A7LAI8
B	277	ALA	PHE	engineered mutation	UNP A7LAI8
B	278	ALA	PRO	engineered mutation	UNP A7LAI8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
			Total	Mg		
2	B	1	1	1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

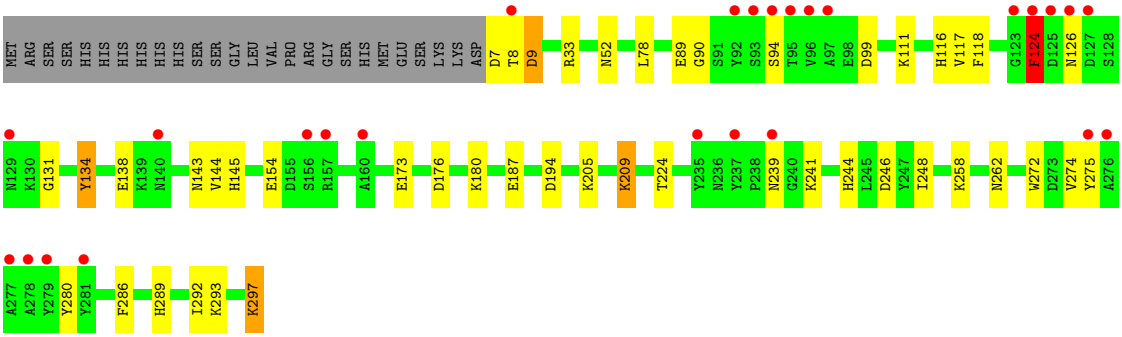
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	240	Total O 240 240	0	0
4	B	232	Total O 232 232	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

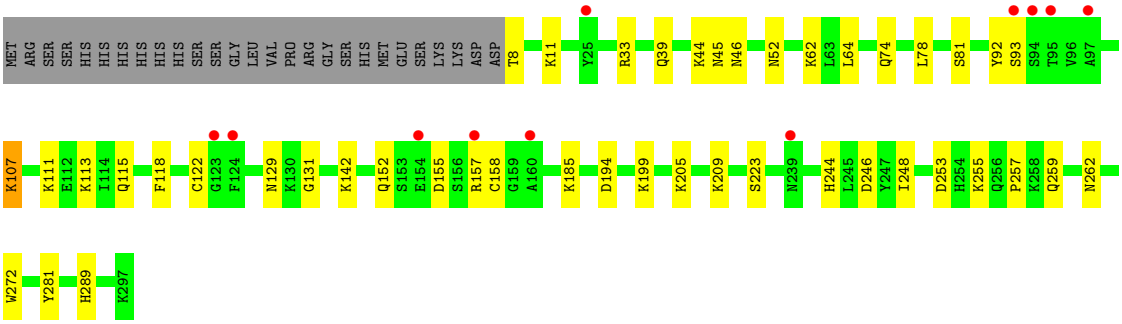
• Molecule 1: Beta-hemolysin

Chain A:



• Molecule 1: Beta-hemolysin

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.90Å 68.58Å 126.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.16 – 1.80 27.88 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.16-1.80) 99.8 (27.88-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.220 0.182 , 0.219	Depositor DCC
R_{free} test set	2625 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5150	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4

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	1/2396 (0.0%)	0.74	1/3242 (0.0%)
1	B	0.66	0/2388	0.70	0/3231
All	All	0.68	1/4784 (0.0%)	0.72	1/6473 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	TYR	CD1-CE1	5.04	1.47	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	9	ASP	CB-CA-C	7.29	124.97	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	PHE	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	2337	0	2251	41	0
1	B	2329	0	2247	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	2	0
3	B	5	0	0	1	0
4	A	240	0	0	10	0
4	B	232	0	0	11	0
All	All	5150	0	4498	71	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 8.

All (71) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LYS:HD2	1:A:138:GLU:HB2	1.42	0.97
1:A:248:ILE:H	1:A:262:ASN:HD21	1.26	0.82
1:B:44:LYS:HE3	4:B:365:HOH:O	1.82	0.80
1:A:111:LYS:NZ	1:A:143:ASN:HD21	1.81	0.79
1:B:248:ILE:H	1:B:262:ASN:HD21	1.38	0.71
1:B:107:LYS:HE3	4:B:440:HOH:O	1.90	0.71
1:A:154:GLU:HG2	4:A:308:HOH:O	1.91	0.70
1:B:246:ASP:OD1	1:B:289:HIS:HD2	1.76	0.69
1:A:116:HIS:HE1	1:A:173:GLU:OE1	1.76	0.68
1:A:111:LYS:HZ2	1:A:143:ASN:HD21	1.41	0.68
1:A:8:THR:HG21	4:A:394:HOH:O	1.94	0.66
1:B:8:THR:HG21	4:B:444:HOH:O	1.96	0.65
1:A:52:ASN:HD21	1:A:194:ASP:H	1.43	0.65
1:B:39:GLN:OE1	4:B:355:HOH:O	2.14	0.65
1:A:248:ILE:H	1:A:262:ASN:ND2	1.95	0.65
1:B:122:CYS:H	1:B:152:GLN:NE2	1.96	0.63
1:A:205:LYS:O	1:A:209:LYS:HD2	1.99	0.63
1:A:246:ASP:OD1	1:A:289:HIS:HD2	1.82	0.62
1:A:145:HIS:HE1	1:A:187:GLU:OE1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:SER:H	1:B:129:ASN:HD21	1.46	0.62
1:A:134:TYR:OH	1:A:145:HIS:HD2	1.83	0.62
1:B:8:THR:N	4:B:330:HOH:O	2.32	0.62
1:A:275:TYR:CE2	1:A:280:TYR:HE1	2.17	0.62
1:B:244:HIS:HE1	4:B:304:HOH:O	1.82	0.61
1:A:289:HIS:HE1	3:A:403:PO4:O2	1.85	0.60
1:A:52:ASN:ND2	1:A:194:ASP:H	2.01	0.59
1:A:124:PHE:N	1:A:124:PHE:CD2	2.71	0.59
1:A:89:GLU:OE2	1:A:116:HIS:HD2	1.86	0.59
1:B:62:LYS:HG2	4:B:492:HOH:O	2.03	0.58
1:A:244:HIS:HE1	4:A:329:HOH:O	1.87	0.58
1:A:176:ASP:HB3	4:A:370:HOH:O	2.04	0.57
1:B:8:THR:CG2	4:B:444:HOH:O	2.53	0.56
1:A:275:TYR:CE2	1:A:280:TYR:CE1	2.94	0.56
1:B:248:ILE:H	1:B:262:ASN:ND2	2.06	0.54
1:B:255:LYS:HE2	4:B:335:HOH:O	2.09	0.53
1:A:297:LYS:OXT	1:B:259:GLN:NE2	2.41	0.53
1:B:157:ARG:NE	1:B:157:ARG:HA	2.25	0.52
1:B:289:HIS:HE1	3:B:404:PO4:O3	1.92	0.52
1:A:111:LYS:HZ2	1:A:143:ASN:ND2	2.04	0.52
1:A:118:PHE:CD2	1:A:131:GLY:HA2	2.45	0.52
1:B:122:CYS:H	1:B:152:GLN:HE22	1.59	0.51
1:B:185:LYS:HD2	1:B:253:ASP:O	2.11	0.51
1:B:118:PHE:CD2	1:B:131:GLY:HA2	2.47	0.50
1:B:52:ASN:HD21	1:B:194:ASP:H	1.58	0.50
1:B:52:ASN:ND2	1:B:194:ASP:H	2.10	0.50
1:B:223:SER:HB3	4:B:327:HOH:O	2.12	0.49
1:B:46:ASN:O	1:B:107:LYS:HE2	2.14	0.47
1:A:33:ARG:HD3	1:A:272:TRP:CZ2	2.49	0.47
1:A:293:LYS:HE2	4:A:382:HOH:O	2.14	0.47
1:A:111:LYS:HZ3	1:A:143:ASN:HD21	1.58	0.47
1:A:8:THR:HG23	4:A:490:HOH:O	2.15	0.45
1:A:180:LYS:CE	4:A:309:HOH:O	2.63	0.45
1:A:224:THR:HG21	1:A:292:ILE:HD11	1.99	0.44
1:A:293:LYS:NZ	4:A:399:HOH:O	2.29	0.44
1:B:33:ARG:HD3	1:B:272:TRP:CZ2	2.52	0.44
1:B:78:LEU:HD12	1:B:115:GLN:HB2	1.99	0.43
1:B:11:LYS:HE2	1:B:45:ASN:O	2.19	0.43
1:A:8:THR:OG1	1:A:144:VAL:HB	2.19	0.43
1:A:116:HIS:CE1	1:A:173:GLU:OE1	2.65	0.42
1:A:33:ARG:HD2	1:A:286:PHE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LYS:HD3	4:A:383:HOH:O	2.20	0.42
1:A:145:HIS:CE1	1:A:187:GLU:OE1	2.69	0.41
1:B:81:SER:HA	1:B:92:TYR:OH	2.20	0.41
1:B:205:LYS:NZ	4:B:410:HOH:O	2.36	0.41
1:A:134:TYR:OH	1:A:145:HIS:CD2	2.69	0.41
1:B:155:ASP:HB3	1:B:158:CYS:SG	2.60	0.41
1:A:90:GLY:HA3	1:A:117:VAL:O	2.20	0.41
1:A:289:HIS:CE1	3:A:403:PO4:O2	2.70	0.41
1:B:64:LEU:HB3	1:B:74:GLN:HE22	1.86	0.41
1:A:258:LYS:HG3	4:A:436:HOH:O	2.21	0.40
1:A:78:LEU:O	1:A:99:ASP:HB2	2.22	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	289/317 (91%)	282 (98%)	7 (2%)	0	100	100
1	B	288/317 (91%)	281 (98%)	7 (2%)	0	100	100
All	All	577/634 (91%)	563 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	258/282 (92%)	248 (96%)	10 (4%)	32	17
1	B	257/282 (91%)	249 (97%)	8 (3%)	40	25
All	All	515/564 (91%)	497 (96%)	18 (4%)	36	21

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	9	ASP
1	A	94	SER
1	A	124	PHE
1	A	126	ASN
1	A	209	LYS
1	A	239	ASN
1	A	241	LYS
1	A	274	VAL
1	A	297	LYS
1	B	107	LYS
1	B	111	LYS
1	B	113	LYS
1	B	142	LYS
1	B	199	LYS
1	B	209	LYS
1	B	257	PRO
1	B	281	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	74	GLN
1	A	116	HIS
1	A	126	ASN
1	A	140	ASN
1	A	143	ASN
1	A	145	HIS
1	A	214	ASN
1	A	239	ASN
1	A	244	HIS
1	A	262	ASN
1	A	289	HIS

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Mol	Chain	Res	Type
1	B	27	ASN
1	B	52	ASN
1	B	74	GLN
1	B	126	ASN
1	B	129	ASN
1	B	152	GLN
1	B	244	HIS
1	B	262	ASN
1	B	289	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	B	404	2	4,4,4	1.09	0	6,6,6	0.82	0
3	PO4	A	403	2	4,4,4	1.05	0	6,6,6	0.81	0

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	PO4	1	0
3	A	403	PO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	291/317 (91%)	0.24	26 (8%)	9	7	15, 24, 46, 58	0
1	B	290/317 (91%)	0.11	11 (3%)	40	35	17, 27, 41, 51	0
All	All	581/634 (91%)	0.18	37 (6%)	19	15	15, 25, 43, 58	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	VAL	7.8
1	A	126	ASN	7.5
1	A	95	THR	7.2
1	A	97	ALA	6.6
1	B	124	PHE	6.2
1	A	127	ASP	6.1
1	A	156	SER	5.9
1	A	125	ASP	5.3
1	A	279	TYR	5.1
1	A	281	TYR	5.0
1	A	94	SER	4.8
1	A	157	ARG	4.7
1	A	239	ASN	4.6
1	A	93	SER	4.5
1	B	239	ASN	4.4
1	A	277	ALA	4.3
1	B	157	ARG	4.1
1	A	129	ASN	3.8
1	B	95	THR	3.6
1	A	278	ALA	3.6
1	A	237	TYR	3.3
1	A	123	GLY	3.1
1	B	160	ALA	2.8
1	B	93	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	94	SER	2.7
1	B	97	ALA	2.6
1	A	160	ALA	2.6
1	A	124	PHE	2.5
1	B	123	GLY	2.4
1	A	140	ASN	2.4
1	A	276	ALA	2.3
1	A	235	TYR	2.3
1	A	92	TYR	2.3
1	B	25	TYR	2.3
1	A	275	TYR	2.2
1	B	154	GLU	2.1
1	A	8	THR	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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
2	MG	A	402	1/1	0.99	0.02	23,23,23,23	0
2	MG	B	401	1/1	0.99	0.04	26,26,26,26	0
3	PO4	A	403	5/5	0.99	0.03	25,26,28,28	0
3	PO4	B	404	5/5	0.99	0.07	28,28,29,30	0

6.5 Other polymers (i)

There are no such residues in this entry.