Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2016 – 04:59 PM EDT

PDB ID	:	5K59
Title	:	Crystal structure of LukGH from Staphylococcus aureus in complex with a neutralising antibody
Authors	:	Welin, M.; Logan, D.T.; Badarau, A.; Mirkina, I.; Zauner, G.; Dolezilkova, I.; Nagy, E.
Deposited on	:	2016-05-23
Resolution	:	2.84 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:

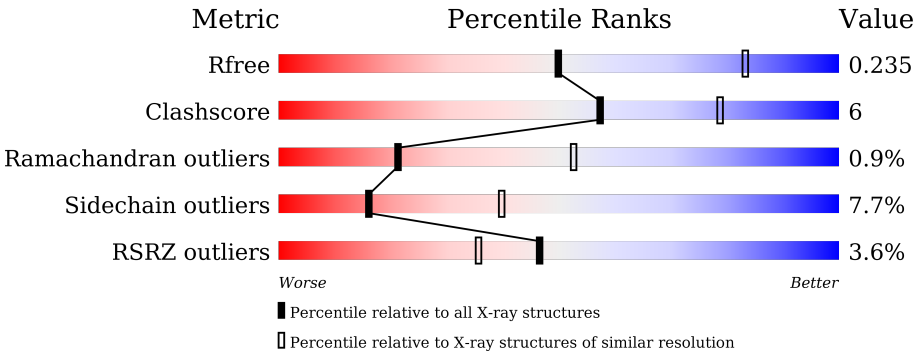
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.84 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	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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 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	C	319	71% 14% • 13%
1	D	319	70% 14% • 14%
2	A	311	80% 12% • 6%
2	B	311	82% 10% • 6%
3	E	227	13% 72% 18% • 7%
3	H	227	8% 69% 20% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	214	8% 81% 15%
4	L	214	79% 16%

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
6	PO4	A	401	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15764 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 Uncharacterized leukocidin-like protein 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	D	275	Total	C	N	O	0	0	0
			2280	1441	395	444			
1	C	276	Total	C	N	O	0	0	0
			2289	1447	397	445			

- Molecule 2 is a protein called Uncharacterized leukocidin-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	293	Total	C	N	O	S	0	0	0
			2383	1492	414	472	5			
2	A	292	Total	C	N	O	S	0	0	0
			2379	1490	413	471	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP Q2FFA3
B	0	LEU	-	expression tag	UNP Q2FFA3
A	-1	SER	-	expression tag	UNP Q2FFA3
A	0	LEU	-	expression tag	UNP Q2FFA3

- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	212	Total	C	N	O	S	0	0	0
			1591	1009	261	315	6			
3	E	210	Total	C	N	O	S	0	0	0
			1572	996	259	311	6			

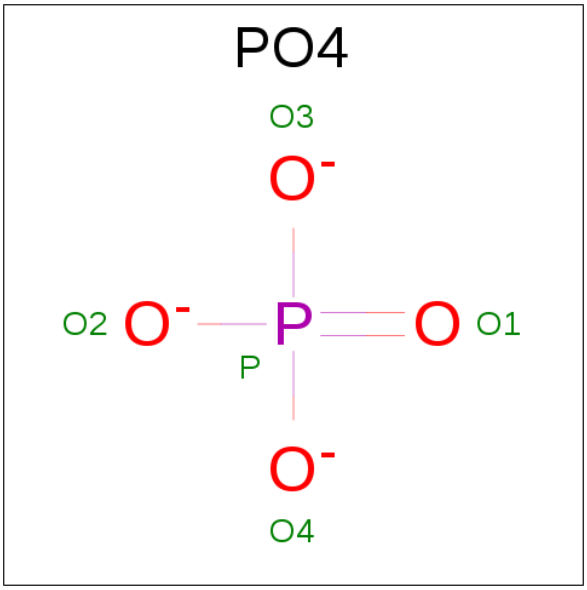
- Molecule 4 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	212	Total	C	N	O	S	0	0	0
			1625	1018	272	330	5			
4	F	212	Total	C	N	O	S	0	0	0
			1625	1018	272	330	5			

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

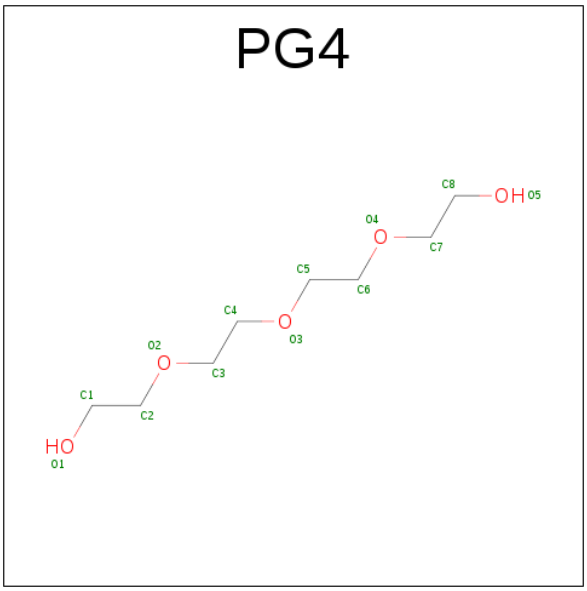
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 10 6 4	0	0

- Molecule 8 is water.

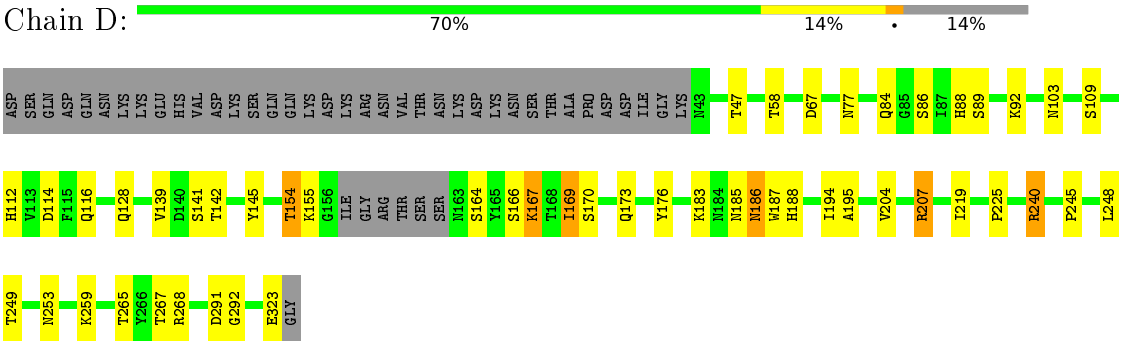
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	2	Total O 2 2	0	0
8	C	1	Total O 1 1	0	0
8	A	1	Total O 1 1	0	0

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.

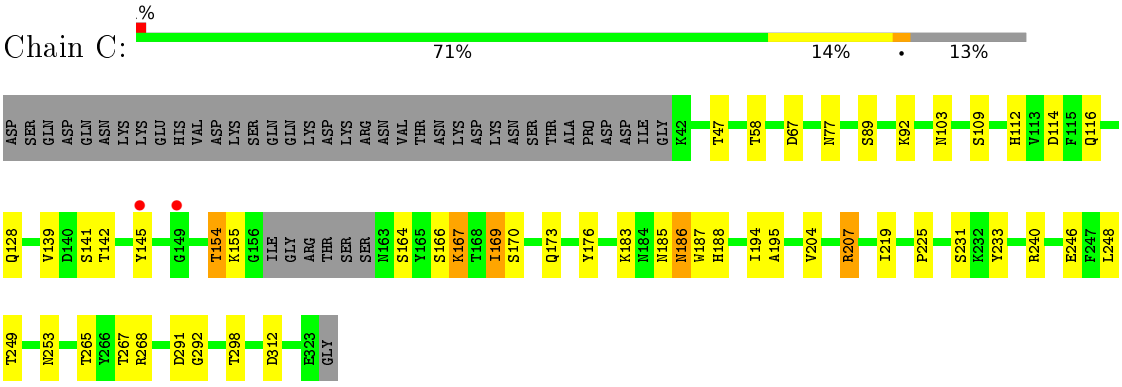
- Molecule 1: Uncharacterized leukocidin-like protein 2

Chain D:



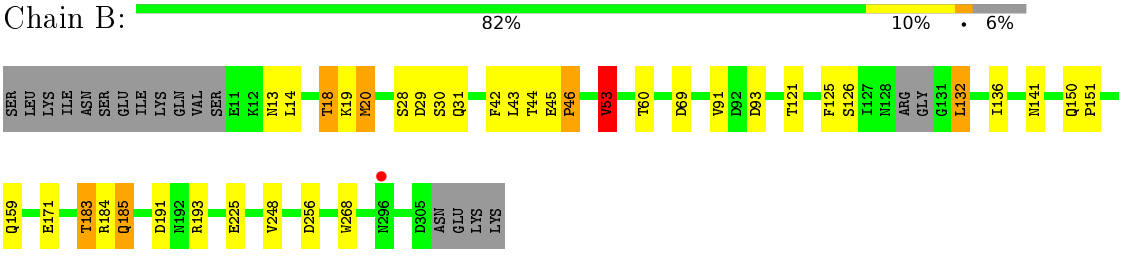
- Molecule 1: Uncharacterized leukocidin-like protein 2

Chain C:

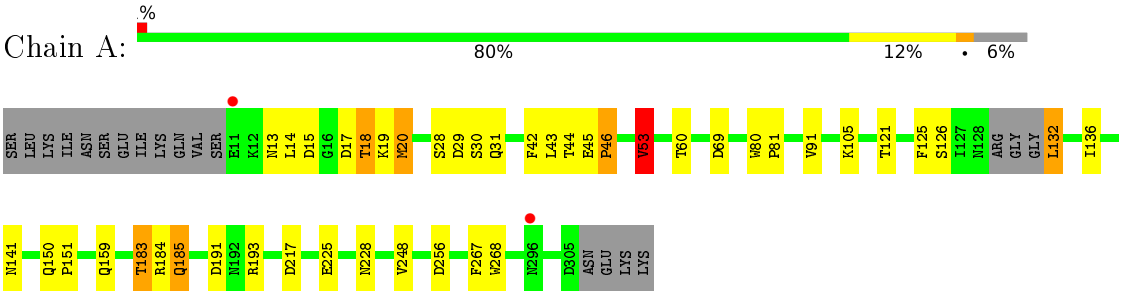


- Molecule 2: Uncharacterized leukocidin-like protein 1

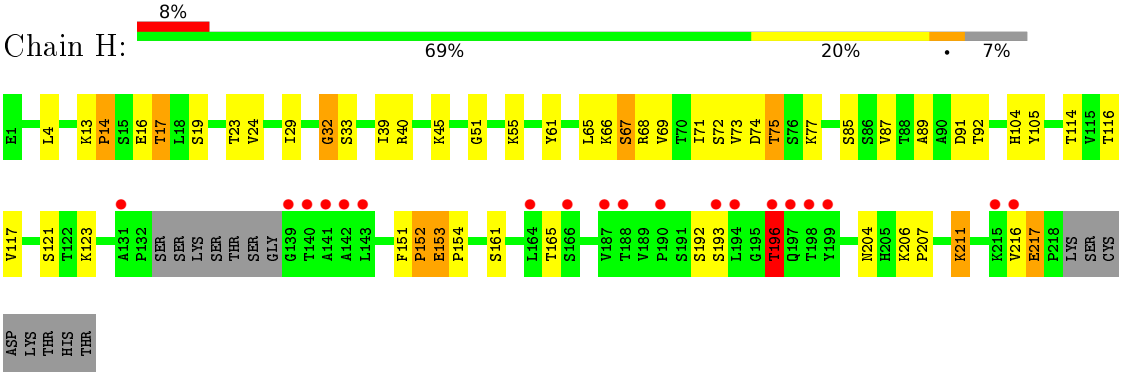
Chain B:



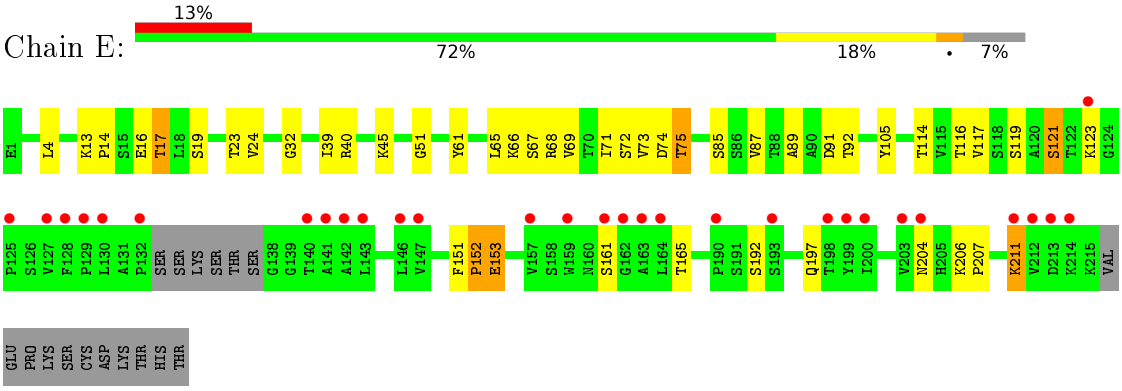
- Molecule 2: Uncharacterized leukocidin-like protein 1



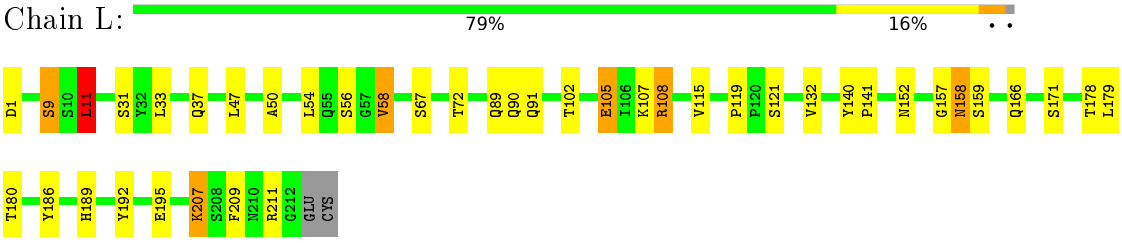
• Molecule 3: Fab heavy chain



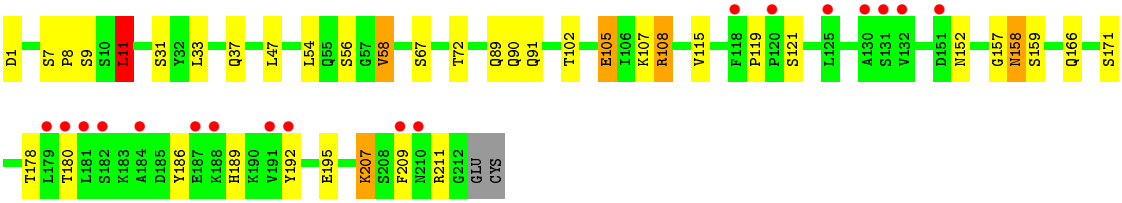
• Molecule 3: Fab heavy chain



• Molecule 4: Fab light chain



• Molecule 4: Fab light chain


D1
S7
P8
S9
S10
L11
S31
Y32
L33
Q37
L47
L54
Q55
S56
G57
V58
S67
T72
Q89
Q90
Q91
T102
E105
I106
K107
R108
V115
F118
P119
P120
S121
L125
A130
S131
V132
D151
N152
G157
N158
S159
Q166
S171
T178
L179
T180
L181
S182
K183
A184
D185
Y186
E187
K188
H189
K190
V191
Y192
E195
K207
S208
F209
N210
R211
G212
GLU
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.79Å 160.93Å 119.48Å 90.00° 101.18° 90.00°	Depositor
Resolution (Å)	48.54 – 2.84 48.49 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.54-2.84) 99.1 (48.49-2.84)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.197 , 0.237 0.201 , 0.235	Depositor DCC
R_{free} test set	3277 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	62.2	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15764	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, PG4, CL

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	C	0.58	0/2340	0.76	0/3158
1	D	0.59	0/2331	0.78	0/3147
2	A	0.63	0/2436	0.77	1/3293 (0.0%)
2	B	0.64	0/2440	0.78	1/3298 (0.0%)
3	E	0.50	0/1611	0.70	0/2197
3	H	0.53	0/1631	0.70	0/2226
4	F	0.52	0/1661	0.72	1/2255 (0.0%)
4	L	0.54	0/1661	0.71	1/2255 (0.0%)
All	All	0.58	0/16111	0.75	4/21829 (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
3	E	0	4
3	H	0	4
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	53	VAL	CB-CA-C	-6.33	99.36	111.40
2	B	53	VAL	CB-CA-C	-5.76	100.45	111.40
4	L	11	LEU	CA-CB-CG	5.68	128.37	115.30
4	F	11	LEU	CA-CB-CG	5.52	128.00	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	151	PHE	Peptide
3	E	152	PRO	Peptide
3	E	32	GLY	Peptide
3	E	51	GLY	Peptide
3	H	151	PHE	Peptide
3	H	152	PRO	Peptide
3	H	32	GLY	Peptide
3	H	51	GLY	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	C	2289	0	2240	26	0
1	D	2280	0	2227	26	0
2	A	2379	0	2260	35	0
2	B	2383	0	2263	31	0
3	E	1572	0	1551	16	0
3	H	1591	0	1570	22	0
4	F	1625	0	1577	18	0
4	L	1625	0	1577	20	0
5	D	1	0	0	0	0
6	A	5	0	0	0	0
7	A	10	0	13	0	0
8	A	1	0	0	0	0
8	B	2	0	0	0	0
8	C	1	0	0	0	0
All	All	15764	0	15278	185	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 6.

All (185) 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:18:THR:CG2	2:A:44:THR:O	1.75	1.32

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:LEU:HD21	2:B:19:LYS:CE	1.63	1.29
2:A:18:THR:HG22	2:A:44:THR:O	1.07	1.21
2:B:14:LEU:HD23	2:B:19:LYS:HG3	1.15	1.08
2:A:14:LEU:HD23	2:A:19:LYS:HG2	1.32	1.08
2:A:18:THR:HG23	2:A:45:GLU:HA	1.35	1.08
4:F:157:GLY:O	4:F:158:ASN:ND2	1.90	1.04
4:L:157:GLY:O	4:L:158:ASN:ND2	1.90	1.04
2:B:14:LEU:HD21	2:B:19:LYS:HE2	1.36	1.03
2:B:14:LEU:CD2	2:B:19:LYS:HG3	1.88	1.02
2:B:14:LEU:HD23	2:B:19:LYS:CG	1.92	0.99
2:B:14:LEU:CD2	2:B:19:LYS:CG	2.43	0.96
2:B:14:LEU:CD2	2:B:19:LYS:CE	2.48	0.92
2:B:14:LEU:HD21	2:B:19:LYS:HE3	1.53	0.88
2:B:14:LEU:CD2	2:B:19:LYS:HE3	2.07	0.85
1:D:58:THR:O	1:D:268:ARG:NH2	2.11	0.83
2:B:18:THR:CG2	2:B:44:THR:O	2.27	0.83
2:A:14:LEU:CD2	2:A:19:LYS:HG2	2.09	0.82
1:C:58:THR:O	1:C:268:ARG:NH2	2.14	0.80
2:B:18:THR:HG22	2:B:44:THR:O	1.81	0.78
1:D:185:ASN:HB3	1:D:187:TRP:H	1.48	0.78
2:A:14:LEU:HD21	2:A:19:LYS:HD3	1.67	0.77
2:B:18:THR:HG23	2:B:45:GLU:HA	1.65	0.76
4:L:189:HIS:O	4:L:211:ARG:NH2	2.20	0.75
1:C:185:ASN:HB3	1:C:187:TRP:H	1.52	0.74
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.67	0.74
4:F:189:HIS:O	4:F:211:ARG:NH2	2.20	0.74
2:A:18:THR:HG23	2:A:44:THR:O	1.85	0.74
4:F:37:GLN:HB2	4:F:47:LEU:HD11	1.67	0.74
2:B:14:LEU:HD21	2:B:19:LYS:CD	2.17	0.73
2:A:18:THR:CG2	2:A:45:GLU:HA	2.17	0.72
1:D:89:SER:OG	2:B:159:GLN:NE2	2.24	0.70
3:H:204:ASN:ND2	3:H:211:LYS:HD3	2.10	0.66
2:B:14:LEU:HD21	2:B:19:LYS:CG	2.20	0.65
2:B:18:THR:HG23	2:B:44:THR:O	1.95	0.65
3:H:77:LYS:HE2	3:E:121:SER:HA	1.78	0.65
4:F:157:GLY:C	4:F:158:ASN:HD22	1.96	0.64
1:C:89:SER:OG	2:A:159:GLN:NE2	2.31	0.64
3:E:204:ASN:ND2	3:E:211:LYS:HD3	2.12	0.63
2:A:184:ARG:HD2	2:A:256:ASP:OD2	1.99	0.63
2:B:184:ARG:HD2	2:B:256:ASP:OD2	2.00	0.62
3:H:13:LYS:HB2	3:H:16:GLU:HG3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:18:THR:HG23	2:A:45:GLU:CA	2.21	0.62
2:A:14:LEU:HD21	2:A:19:LYS:CD	2.29	0.61
1:D:154:THR:OG1	1:D:155:LYS:N	2.34	0.61
3:H:204:ASN:HD22	3:H:211:LYS:HD3	1.65	0.61
3:E:204:ASN:HD22	3:E:211:LYS:HD3	1.66	0.59
1:C:154:THR:OG1	1:C:155:LYS:N	2.37	0.58
4:F:89:GLN:HE22	4:F:91:GLN:CG	2.17	0.58
4:F:54:LEU:HG	4:F:58:VAL:HG22	1.85	0.58
2:A:121:THR:HG23	2:A:141:ASN:HD22	1.69	0.58
2:B:121:THR:HG23	2:B:141:ASN:HD22	1.70	0.57
4:L:89:GLN:HE22	4:L:91:GLN:CG	2.17	0.57
4:L:54:LEU:HG	4:L:58:VAL:HG22	1.85	0.57
3:H:77:LYS:NZ	3:E:119:SER:O	2.37	0.56
3:E:4:LEU:HD22	3:E:24:VAL:HG22	1.88	0.56
2:A:18:THR:CG2	2:A:44:THR:C	2.71	0.55
4:L:119:PRO:HB3	4:L:209:PHE:CE2	2.42	0.55
4:L:157:GLY:C	4:L:158:ASN:HD22	1.98	0.55
2:A:121:THR:H	2:A:141:ASN:ND2	2.04	0.55
3:H:4:LEU:HD22	3:H:24:VAL:HG22	1.88	0.55
2:B:125:PHE:CE2	2:B:132:LEU:HD11	2.42	0.54
2:B:14:LEU:CD2	2:B:19:LYS:HG2	2.36	0.54
2:B:18:THR:HG23	2:B:45:GLU:CA	2.37	0.53
4:F:119:PRO:HB3	4:F:209:PHE:CE2	2.42	0.53
2:A:14:LEU:HD23	2:A:19:LYS:CG	2.21	0.53
3:H:216:VAL:O	3:H:217:GLU:HB3	2.08	0.52
3:H:68:ARG:HH22	3:H:91:ASP:CG	2.12	0.52
1:D:240:ARG:NH2	2:B:171:GLU:OE1	2.41	0.52
1:D:186:ASN:OD1	1:D:186:ASN:N	2.43	0.52
2:A:42:PHE:CD2	2:A:53:VAL:HG13	2.45	0.51
3:E:13:LYS:HB2	3:E:16:GLU:HG3	1.91	0.51
3:E:68:ARG:HH22	3:E:91:ASP:CG	2.14	0.51
2:A:125:PHE:CE2	2:A:132:LEU:HD11	2.45	0.51
2:A:14:LEU:CD2	2:A:19:LYS:CG	2.85	0.51
2:B:121:THR:H	2:B:141:ASN:ND2	2.08	0.51
1:D:139:VAL:O	1:D:170:SER:HA	2.11	0.51
3:E:65:LEU:O	3:E:67:SER:N	2.44	0.51
2:A:18:THR:CG2	2:A:45:GLU:CA	2.87	0.50
1:C:139:VAL:O	1:C:170:SER:HA	2.12	0.50
1:D:67:ASP:OD2	1:D:167:LYS:HE2	2.12	0.50
2:A:91:VAL:HG11	2:A:248:VAL:HG23	1.94	0.50
2:B:91:VAL:HG11	2:B:248:VAL:HG23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:TYR:O	1:C:164:SER:HB2	2.12	0.50
1:C:103:ASN:ND2	1:C:225:PRO:HA	2.26	0.50
1:D:77:ASN:HD22	1:D:253:ASN:HD22	1.60	0.49
1:C:67:ASP:OD2	1:C:167:LYS:HE2	2.13	0.49
1:C:128:GLN:HB2	1:C:249:THR:HG22	1.94	0.49
1:C:77:ASN:HD22	1:C:253:ASN:HD22	1.60	0.49
1:D:128:GLN:HB2	1:D:249:THR:HG22	1.95	0.48
1:D:116:GLN:CG	1:D:188:HIS:HD2	2.27	0.48
4:F:115:VAL:HB	4:F:207:LYS:HG3	1.95	0.48
2:B:42:PHE:CD2	2:B:53:VAL:HG13	2.49	0.48
3:E:17:THR:HB	3:E:85:SER:HA	1.96	0.48
1:C:116:GLN:CG	1:C:188:HIS:HD2	2.27	0.48
1:C:173:GLN:O	1:C:173:GLN:HG2	2.13	0.48
1:D:173:GLN:HG2	1:D:173:GLN:O	2.14	0.48
3:H:65:LEU:O	3:H:67:SER:N	2.47	0.47
3:H:17:THR:HB	3:H:85:SER:HA	1.96	0.47
1:D:145:TYR:O	1:D:164:SER:HB2	2.14	0.47
4:F:186:TYR:HA	4:F:192:TYR:OH	2.14	0.47
2:A:14:LEU:CD2	2:A:19:LYS:CD	2.93	0.47
3:H:32:GLY:HA2	3:H:55:LYS:NZ	2.30	0.47
2:A:15:ASP:N	2:A:18:THR:O	2.28	0.47
1:D:103:ASN:ND2	1:D:225:PRO:HA	2.29	0.47
4:L:186:TYR:HA	4:L:192:TYR:OH	2.15	0.47
4:L:115:VAL:HB	4:L:207:LYS:HG3	1.97	0.47
1:D:88:HIS:O	1:D:268:ARG:NH1	2.47	0.46
1:C:114:ASP:HB3	1:C:265:THR:HB	1.97	0.46
2:A:18:THR:HG21	2:A:45:GLU:HB3	1.98	0.46
4:F:89:GLN:HE22	4:F:91:GLN:HG2	1.79	0.46
1:C:186:ASN:N	1:C:186:ASN:OD1	2.49	0.46
4:F:11:LEU:C	4:F:11:LEU:HD23	2.36	0.46
3:H:206:LYS:HB2	3:H:207:PRO:HD3	1.98	0.46
3:H:216:VAL:O	3:H:217:GLU:CB	2.64	0.46
2:B:13:ASN:OD1	2:B:14:LEU:N	2.49	0.45
2:A:20:MET:HB3	2:A:43:LEU:HD12	1.99	0.45
4:L:11:LEU:C	4:L:11:LEU:HD23	2.37	0.45
2:A:14:LEU:CD2	2:A:19:LYS:HD3	2.44	0.45
1:D:114:ASP:HB3	1:D:265:THR:HB	1.99	0.45
1:C:112:HIS:HB2	1:C:267:THR:HB	1.98	0.45
1:C:291:ASP:OD1	1:C:292:GLY:N	2.49	0.45
1:D:176:TYR:CE2	1:D:195:ALA:HB2	2.52	0.45
1:C:246:GLU:OE1	2:A:105:LYS:HE2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:HIS:HB2	1:D:267:THR:HB	1.98	0.45
4:F:108:ARG:HG3	4:F:171:SER:HB2	1.99	0.44
3:H:152:PRO:HB2	3:H:153:GLU:O	2.17	0.44
2:B:45:GLU:HB2	2:B:46:PRO:CD	2.48	0.44
1:C:169:ILE:HD13	1:C:248:LEU:HD12	1.99	0.44
3:H:89:ALA:O	3:H:92:THR:HG22	2.17	0.44
2:A:183:THR:CG2	2:A:185:GLN:H	2.31	0.44
2:A:45:GLU:HB2	2:A:46:PRO:CD	2.48	0.44
3:E:89:ALA:O	3:E:92:THR:HG22	2.17	0.44
4:L:89:GLN:HE22	4:L:91:GLN:HG2	1.81	0.44
4:L:108:ARG:HG3	4:L:171:SER:HB2	1.99	0.44
3:E:105:TYR:HA	4:F:91:GLN:NE2	2.32	0.44
3:H:61:TYR:HE1	3:H:71:ILE:HG13	1.82	0.44
3:H:105:TYR:HA	4:L:91:GLN:NE2	2.32	0.44
1:D:169:ILE:HD13	1:D:248:LEU:HD12	2.00	0.44
3:E:74:ASP:O	3:E:75:THR:C	2.55	0.44
1:C:176:TYR:CE2	1:C:195:ALA:HB2	2.52	0.44
1:D:109:SER:OG	1:D:207:ARG:NH2	2.51	0.43
3:E:152:PRO:CB	3:E:153:GLU:HB2	2.48	0.43
4:F:105:GLU:HG2	4:F:166:GLN:OE1	2.18	0.43
2:B:183:THR:CG2	2:B:185:GLN:H	2.31	0.43
3:H:74:ASP:O	3:H:75:THR:C	2.56	0.43
1:D:185:ASN:CB	1:D:187:TRP:H	2.24	0.43
2:B:20:MET:HB3	2:B:43:LEU:HD12	2.01	0.43
2:A:150:GLN:N	2:A:151:PRO:CD	2.81	0.43
3:H:152:PRO:CB	3:H:153:GLU:HB2	2.48	0.43
3:E:206:LYS:HB2	3:E:207:PRO:HD3	2.01	0.42
4:L:9:SER:O	4:L:102:THR:HA	2.19	0.42
4:F:9:SER:O	4:F:102:THR:HA	2.19	0.42
1:C:219:ILE:HD12	1:C:219:ILE:O	2.20	0.42
3:E:61:TYR:HE1	3:E:71:ILE:HG13	1.83	0.42
4:F:7:SER:HB2	4:F:8:PRO:HA	2.00	0.42
1:C:194:ILE:HG22	1:C:195:ALA:O	2.20	0.42
3:E:152:PRO:HB2	3:E:153:GLU:O	2.19	0.42
4:L:105:GLU:HG2	4:L:166:GLN:OE1	2.20	0.42
1:C:298:THR:HB	1:C:312:ASP:HB3	2.02	0.42
2:A:80:TRP:HB2	2:A:81:PRO:HD2	2.02	0.42
1:D:291:ASP:OD1	1:D:292:GLY:N	2.53	0.42
3:H:193:SER:HA	3:H:196:THR:OG1	2.20	0.42
1:D:185:ASN:HB3	1:D:187:TRP:N	2.27	0.41
2:B:150:GLN:N	2:B:151:PRO:CD	2.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:ILE:HG22	1:D:195:ALA:O	2.20	0.41
3:H:153:GLU:HA	3:H:154:PRO:HA	1.84	0.41
1:C:109:SER:OG	1:C:207:ARG:NH2	2.53	0.41
2:A:60:THR:OG1	2:A:228:ASN:ND2	2.53	0.41
2:A:267:PHE:CE1	4:L:50:ALA:HB2	2.56	0.41
1:C:77:ASN:HB2	1:C:253:ASN:HB3	2.02	0.41
4:L:159:SER:HA	4:L:178:THR:O	2.20	0.41
1:C:185:ASN:CB	1:C:187:TRP:H	2.25	0.41
1:C:231:SER:HG	1:C:233:TYR:HD2	1.66	0.41
1:D:84:GLN:HA	1:D:245:PRO:O	2.20	0.41
4:F:159:SER:HA	4:F:178:THR:O	2.21	0.41
4:L:132:VAL:HG23	4:L:179:LEU:HB3	2.03	0.41
4:L:140:TYR:CG	4:L:141:PRO:HA	2.56	0.41
2:A:13:ASN:O	2:A:14:LEU:HG	2.22	0.40
1:D:219:ILE:HD12	1:D:219:ILE:O	2.21	0.40
4:L:89:GLN:HE22	4:L:91:GLN:HG3	1.85	0.40
2:B:29:ASP:OD1	2:B:31:GLN:HB3	2.21	0.40
2:A:29:ASP:OD1	2:A:31:GLN:HB3	2.21	0.40
4:F:89:GLN:NE2	4:F:91:GLN:HG2	2.36	0.40
3:H:104:HIS:HB3	3:H:105: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	C	272/319 (85%)	263 (97%)	9 (3%)	0	100	100
1	D	271/319 (85%)	262 (97%)	9 (3%)	0	100	100
2	A	288/311 (93%)	269 (93%)	17 (6%)	2 (1%)	26	59
2	B	289/311 (93%)	269 (93%)	18 (6%)	2 (1%)	26	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	E	206/227 (91%)	190 (92%)	11 (5%)	5 (2%)	7 23
3	H	208/227 (92%)	189 (91%)	10 (5%)	9 (4%)	3 10
4	F	210/214 (98%)	199 (95%)	11 (5%)	0	100 100
4	L	210/214 (98%)	199 (95%)	11 (5%)	0	100 100
All	All	1954/2142 (91%)	1840 (94%)	96 (5%)	18 (1%)	21 52

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	14	PRO
3	H	66	LYS
3	H	217	GLU
3	E	14	PRO
3	E	66	LYS
2	B	136	ILE
2	A	136	ILE
3	H	33	SER
3	H	196	THR
3	E	75	THR
3	H	75	THR
3	H	192	SER
3	E	192	SER
2	B	46	PRO
3	H	153	GLU
2	A	46	PRO
3	H	29	ILE
3	E	153	GLU

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	C	258/297 (87%)	245 (95%)	13 (5%)	30 62
1	D	257/297 (86%)	241 (94%)	16 (6%)	23 52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	266/283 (94%)	250 (94%)	16 (6%)	24 54
2	B	266/283 (94%)	250 (94%)	16 (6%)	24 54
3	E	180/197 (91%)	161 (89%)	19 (11%)	8 23
3	H	183/197 (93%)	162 (88%)	21 (12%)	7 19
4	F	186/188 (99%)	168 (90%)	18 (10%)	10 27
4	L	186/188 (99%)	167 (90%)	19 (10%)	9 25
All	All	1782/1930 (92%)	1644 (92%)	138 (8%)	16 40

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	47	THR
1	D	86	SER
1	D	92	LYS
1	D	141	SER
1	D	142	THR
1	D	154	THR
1	D	166	SER
1	D	167	LYS
1	D	169	ILE
1	D	183	LYS
1	D	186	ASN
1	D	204	VAL
1	D	207	ARG
1	D	240	ARG
1	D	259	LYS
1	D	323	GLU
2	B	18	THR
2	B	20	MET
2	B	28	SER
2	B	30	SER
2	B	53	VAL
2	B	60	THR
2	B	69	ASP
2	B	93	ASP
2	B	126	SER
2	B	132	LEU
2	B	183	THR
2	B	185	GLN
2	B	191	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	193	ARG
2	B	225	GLU
2	B	268	TRP
1	C	47	THR
1	C	92	LYS
1	C	141	SER
1	C	142	THR
1	C	154	THR
1	C	166	SER
1	C	167	LYS
1	C	169	ILE
1	C	183	LYS
1	C	186	ASN
1	C	204	VAL
1	C	207	ARG
1	C	240	ARG
2	A	17	ASP
2	A	18	THR
2	A	20	MET
2	A	28	SER
2	A	30	SER
2	A	53	VAL
2	A	69	ASP
2	A	126	SER
2	A	132	LEU
2	A	183	THR
2	A	185	GLN
2	A	191	ASP
2	A	193	ARG
2	A	217	ASP
2	A	225	GLU
2	A	268	TRP
3	H	14	PRO
3	H	17	THR
3	H	19	SER
3	H	23	THR
3	H	39	ILE
3	H	40	ARG
3	H	45	LYS
3	H	67	SER
3	H	69	VAL
3	H	72	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	73	VAL
3	H	87	VAL
3	H	114	THR
3	H	116	THR
3	H	117	VAL
3	H	121	SER
3	H	123	LYS
3	H	161	SER
3	H	165	THR
3	H	196	THR
3	H	211	LYS
4	L	1	ASP
4	L	9	SER
4	L	11	LEU
4	L	31	SER
4	L	33	LEU
4	L	56	SER
4	L	58	VAL
4	L	67	SER
4	L	72	THR
4	L	90	GLN
4	L	105	GLU
4	L	107	LYS
4	L	108	ARG
4	L	121	SER
4	L	152	ASN
4	L	158	ASN
4	L	180	THR
4	L	195	GLU
4	L	207	LYS
3	E	17	THR
3	E	19	SER
3	E	23	THR
3	E	39	ILE
3	E	40	ARG
3	E	45	LYS
3	E	69	VAL
3	E	72	SER
3	E	73	VAL
3	E	87	VAL
3	E	114	THR
3	E	116	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	117	VAL
3	E	121	SER
3	E	123	LYS
3	E	161	SER
3	E	165	THR
3	E	197	GLN
3	E	211	LYS
4	F	1	ASP
4	F	11	LEU
4	F	31	SER
4	F	33	LEU
4	F	56	SER
4	F	58	VAL
4	F	67	SER
4	F	72	THR
4	F	90	GLN
4	F	105	GLU
4	F	107	LYS
4	F	108	ARG
4	F	121	SER
4	F	152	ASN
4	F	158	ASN
4	F	180	THR
4	F	195	GLU
4	F	207	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	63	ASN
1	D	77	ASN
1	D	188	HIS
1	D	318	ASN
2	B	95	ASN
2	B	141	ASN
2	B	159	GLN
2	B	228	ASN
1	C	63	ASN
1	C	77	ASN
1	C	188	HIS
1	C	318	ASN
2	A	95	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	141	ASN
2	A	159	GLN
2	A	228	ASN
3	H	204	ASN
3	E	204	ASN

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 3 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
6	PO4	A	401	-	4,4,4	0.38	0	6,6,6	0.25	0
7	PG4	A	402	-	9,9,12	0.65	0	8,8,11	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PO4	A	401	-	-	0/0/0/0	0/0/0/0
7	PG4	A	402	-	-	0/7/7/10	0/0/0/0

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.

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 (i)

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	C	276/319 (86%)	-0.15	2 (0%) 89 85	42, 65, 93, 104	0
1	D	275/319 (86%)	-0.15	0 100 100	36, 63, 92, 110	0
2	A	292/311 (93%)	-0.29	2 (0%) 89 85	42, 59, 90, 126	0
2	B	293/311 (94%)	-0.26	1 (0%) 94 92	37, 60, 90, 119	0
3	E	210/227 (92%)	0.49	30 (14%) 4 2	57, 100, 154, 180	0
3	H	212/227 (93%)	0.12	19 (8%) 12 6	51, 78, 120, 150	0
4	F	212/214 (99%)	0.30	18 (8%) 13 7	52, 81, 168, 193	0
4	L	212/214 (99%)	-0.06	0 100 100	46, 73, 111, 120	0
All	All	1982/2142 (92%)	-0.03	72 (3%) 46 36	36, 68, 135, 193	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	193	SER	6.4
3	H	193	SER	5.4
4	F	192	TYR	5.4
4	F	184	ALA	5.2
4	F	182	SER	4.7
4	F	181	LEU	4.7
3	E	203	VAL	4.2
3	E	128	PHE	4.1
4	F	130	ALA	4.1
3	E	129	PRO	4.1
3	H	190	PRO	3.9
3	E	127	VAL	3.8
3	E	141	ALA	3.8
4	F	191	VAL	3.8
3	E	159	TRP	3.7
3	H	198	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	142	ALA	3.4
3	E	132	PRO	3.4
3	E	125	PRO	3.4
4	F	120	PRO	3.4
3	H	199	TYR	3.3
3	H	143	LEU	3.2
3	E	212	VAL	3.2
3	E	146	LEU	3.1
4	F	180	THR	3.1
3	E	199	TYR	3.1
4	F	125	LEU	3.1
3	E	163	ALA	3.1
3	E	143	LEU	3.0
4	F	131	SER	3.0
3	E	204	ASN	3.0
3	H	196	THR	3.0
3	H	216	VAL	2.9
3	E	161	SER	2.8
4	F	188	LYS	2.8
3	H	194	LEU	2.8
4	F	187	GLU	2.8
3	E	213	ASP	2.7
3	E	130	LEU	2.7
3	H	197	GLN	2.7
3	E	200	ILE	2.7
4	F	151	ASP	2.7
3	H	141	ALA	2.6
3	H	187	VAL	2.6
3	E	123	LYS	2.5
1	C	145	TYR	2.5
2	B	296	ASN	2.5
4	F	210	ASN	2.5
2	A	11	GLU	2.5
3	E	211	LYS	2.5
3	H	188	THR	2.5
3	E	164	LEU	2.5
4	F	209	PHE	2.4
3	H	166	SER	2.3
4	F	118	PHE	2.3
2	A	296	ASN	2.3
3	E	157	VAL	2.3
3	E	147	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	179	LEU	2.2
3	E	214	LYS	2.2
3	H	164	LEU	2.2
3	H	215	LYS	2.2
4	F	132	VAL	2.2
3	H	139	GLY	2.1
3	H	131	ALA	2.1
3	E	190	PRO	2.1
3	H	140	THR	2.1
3	E	162	GLY	2.1
3	H	142	ALA	2.0
3	E	140	THR	2.0
3	E	198	THR	2.0
1	C	149	GLY	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	PO4	A	401	5/5	0.82	0.38	9.07	81,86,111,126	0
7	PG4	A	402	10/13	0.94	0.19	1.60	59,64,69,70	0
5	CL	D	401	1/1	0.98	0.11	-1.75	74,74,74,74	0

6.5 Other polymers (i)

There are no such residues in this entry.