



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:13 PM UTC

PDB ID : 5K59 / pdb_00005k59
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

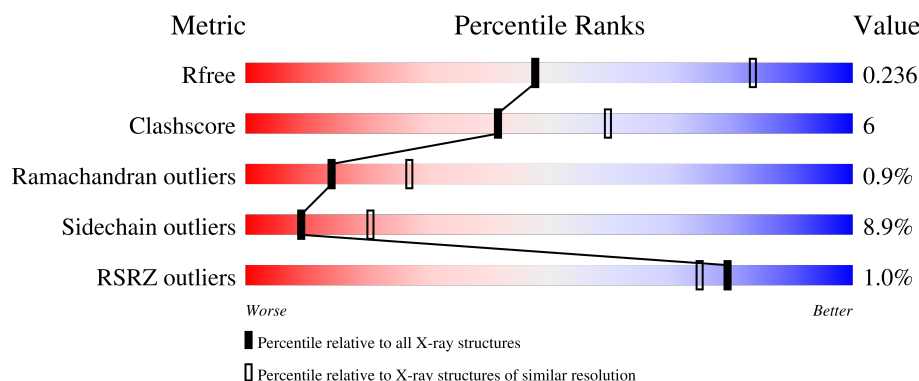
1 Overall quality at a glance

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}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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 $\leq 5\%$. 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	% 70% 14% • 13%
1	D	319	% 70% 14% • 14%
2	A	311	77% 14% •• 6%
2	B	311	79% 12% •• 6%
3	E	227	% 69% 19% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	227	67% 22% • • 7%
4	F	214	3% 79% 18% • •
4	L	214	% 78% 19% • •

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			

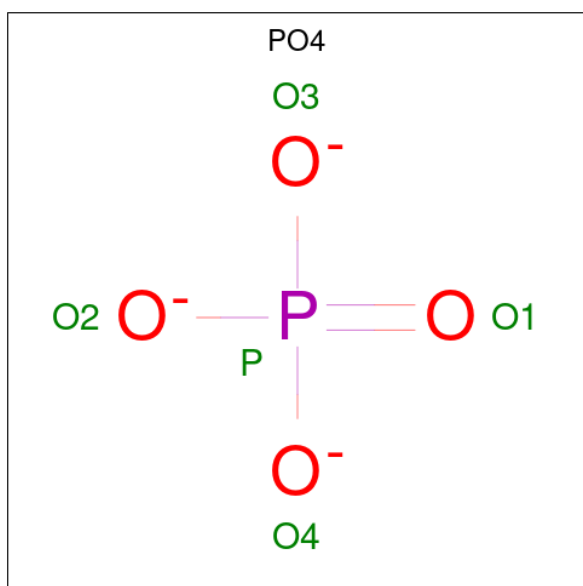
- Molecule 4 is a protein called Fab light chain.

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 (CCD ID: CL) (formula: Cl).

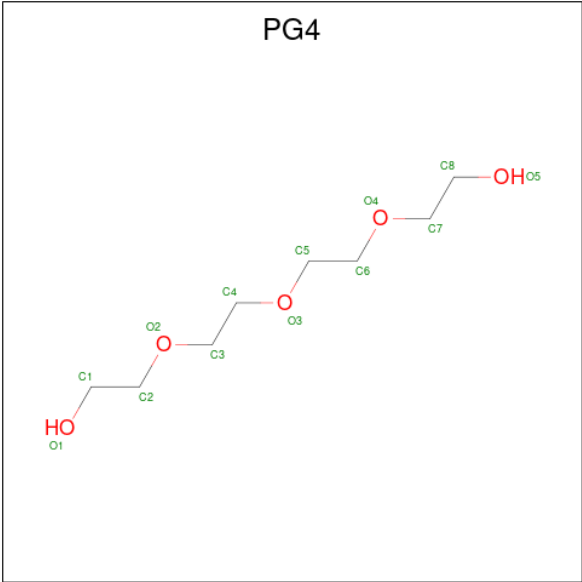
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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

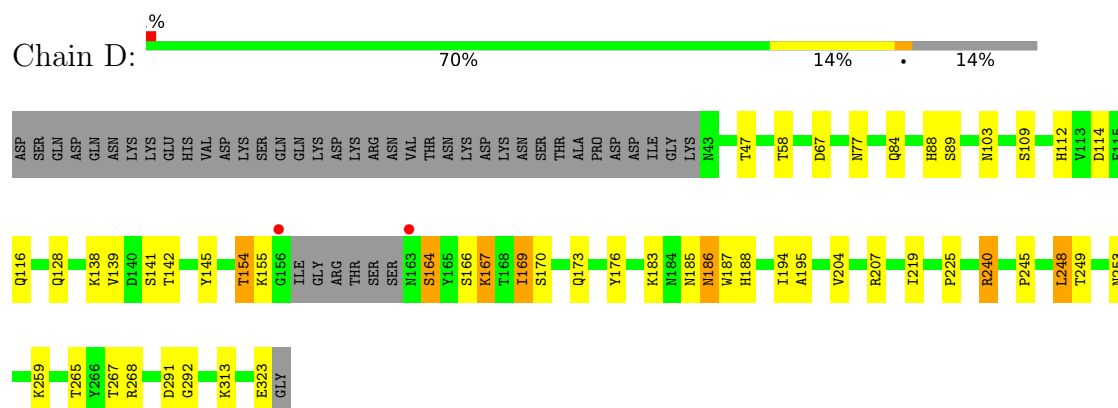
- Molecule 8 is water.

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

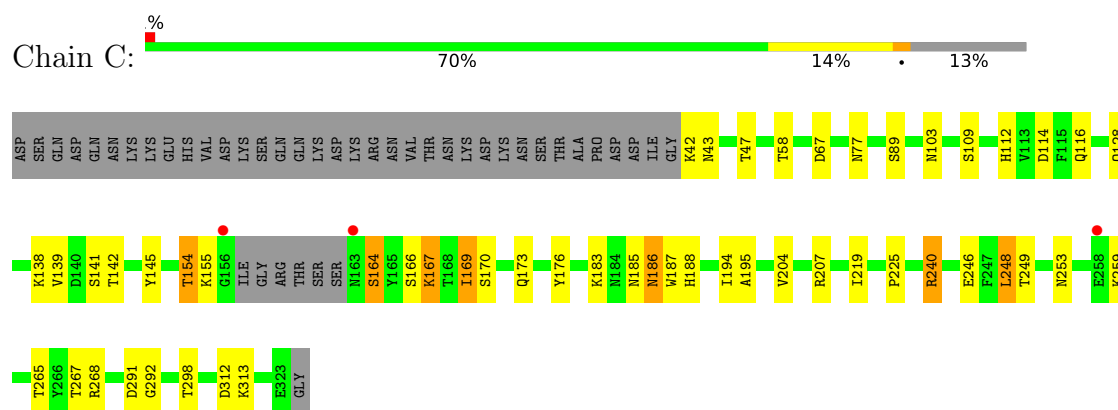
3 Residue-property plots [i](#)

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.

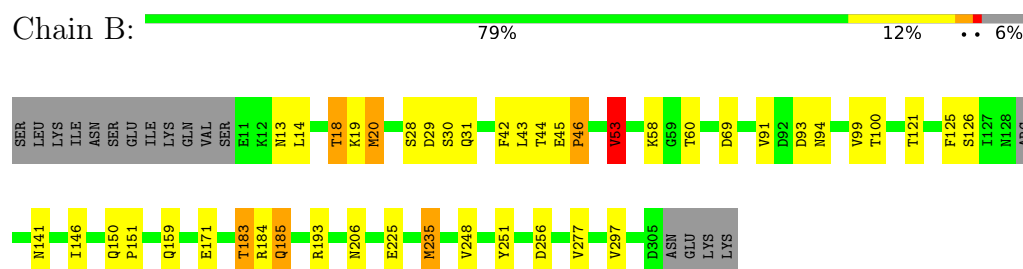
- Molecule 1: Uncharacterized leukocidin-like protein 2



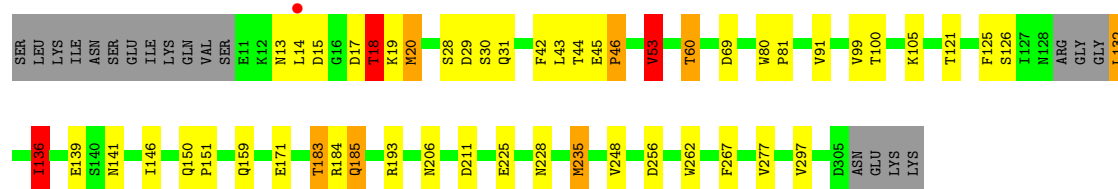
- Molecule 1: Uncharacterized leukocidin-like protein 2



- Molecule 2: Uncharacterized leukocidin-like protein 1

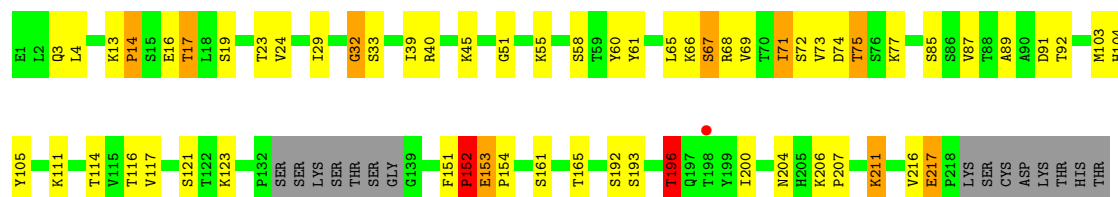


Chain A:  77% 14% 6%



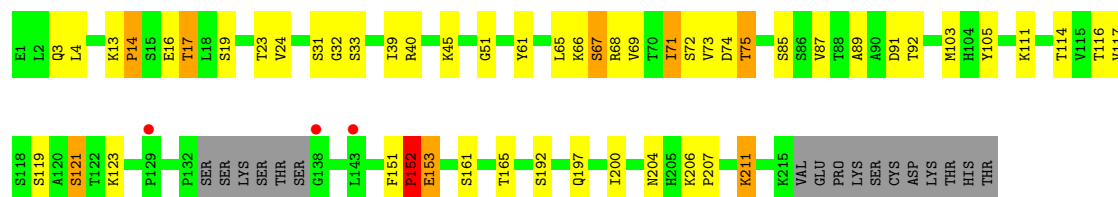
• Molecule 3: Fab heavy chain

Chain H:  67% 22% 7%



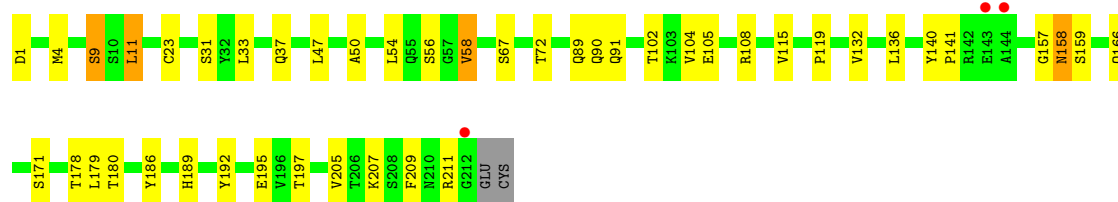
• Molecule 3: Fab heavy chain

Chain E:  69% 19% 7%



• Molecule 4: Fab light chain

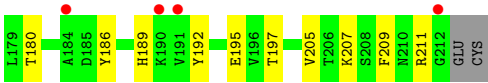
Chain L:  78% 19% 2%



• Molecule 4: Fab light chain

Chain F:  79% 18% 3%





4 Data and refinement statistics

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 48.54 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.54-2.84) 99.1 (48.54-2.84)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.197 , 0.237 0.201 , 0.236	Depositor DCC
R_{free} test set	3277 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PG4, PO4, 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	0.77	0/2340	0.94	1/3158 (0.0%)
1	D	0.78	0/2331	0.96	1/3147 (0.0%)
2	A	0.81	0/2436	0.94	3/3293 (0.1%)
2	B	0.85	0/2440	0.95	3/3298 (0.1%)
3	E	0.68	0/1611	0.92	4/2197 (0.2%)
3	H	0.71	0/1631	0.89	2/2226 (0.1%)
4	F	0.71	0/1661	0.91	0/2255
4	L	0.72	0/1661	0.91	0/2255
All	All	0.77	0/16111	0.93	14/21829 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	4
3	H	0	4
All	All	0	8

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	33	SER	N-CA-C	-8.13	103.45	112.72
2	A	53	VAL	CB-CA-C	-7.44	99.36	110.82
1	D	164	SER	N-CA-C	7.19	118.09	108.38
2	B	53	VAL	CB-CA-C	-6.74	100.45	110.82
3	E	31	SER	N-CA-C	-5.96	105.86	113.01
1	C	164	SER	N-CA-C	5.85	116.28	108.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	152	PRO	CA-C-N	5.75	132.04	121.70
3	H	152	PRO	C-N-CA	5.75	132.04	121.70
3	E	152	PRO	CA-C-N	5.52	131.64	121.70
3	E	152	PRO	C-N-CA	5.52	131.64	121.70
2	B	94	ASN	N-CA-C	5.45	117.36	110.33
2	B	136	ILE	N-CA-C	5.42	120.61	109.34
2	A	18	THR	N-CA-C	5.20	118.03	109.72
2	A	136	ILE	N-CA-C	5.18	120.12	109.34

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	27	0
2	A	2379	0	2260	42	0
2	B	2383	0	2263	36	0
3	E	1572	0	1551	17	0
3	H	1591	0	1570	27	0
4	F	1625	0	1577	19	0
4	L	1625	0	1577	21	0
5	D	1	0	0	0	0
6	A	5	0	0	0	0
7	A	10	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	199	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 (199) 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
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:L:157:GLY:O	4:L:158:ASN:ND2	1.90	1.04
4:F:157:GLY:O	4:F: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:F:157:GLY:C	4:F:158:ASN:HD22	1.96	0.69
4:L:157:GLY:C	4:L:158:ASN:HD22	1.98	0.67
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:A:262:TRP:CZ2	3:H:103:MET:HE1	2.31	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
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
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
2:A:18:THR:CG2	2:A:44:THR:C	2.71	0.60
3:E:204:ASN:HD22	3:E:211:LYS:HD3	1.66	0.59
4:F:4:MET:HE3	4:F:23:CYS:SG	2.43	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
3:H:68:ARG:HH22	3:H:91:ASP:CG	2.12	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:E:4:LEU:HD22	3:E:24:VAL:HG22	1.88	0.56
3:E:68:ARG:HH22	3:E:91:ASP:CG	2.14	0.55
4:L:4:MET:HE3	4:L:23:CYS:SG	2.47	0.55
4:L:119:PRO:HB3	4:L:209:PHE:CE2	2.42	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:14:LEU:CD2	2:B:19:LYS:HG2	2.36	0.54
2:B:125:PHE:CE2	2:B:132:LEU:HD11	2.42	0.54
2:B:206:ASN:HA	3:E:103:MET:HE2	1.90	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:206:ASN:HA	3:H:103:MET:HE2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:240:ARG:NH2	2:B:171:GLU:OE1	2.41	0.52
1:D:186:ASN:N	1:D:186:ASN:OD1	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
4:F:11:LEU:C	4:F:11:LEU:HD23	2.36	0.51
1:D:139:VAL:O	1:D:170:SER:HA	2.11	0.51
2:B:121:THR:H	2:B:141:ASN:ND2	2.08	0.51
2:A:14:LEU:CD2	2:A:19:LYS:CG	2.85	0.51
2:A:125:PHE:CE2	2:A:132:LEU:HD11	2.45	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
4:L:11:LEU:HD23	4:L:11:LEU:C	2.37	0.50
1:C:103:ASN:ND2	1:C:225:PRO:HA	2.26	0.50
1:C:145:TYR:O	1:C:164:SER:HB2	2.12	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:77:ASN:HD22	1:C:253:ASN:HD22	1.60	0.49
1:C:128:GLN:HB2	1:C:249:THR:HG22	1.94	0.49
2:B:58:LYS:O	2:B:251:TYR:OH	2.22	0.49
2:A:262:TRP:CH2	3:H:103:MET:HE1	2.47	0.49
3:E:74:ASP:O	3:E:75:THR:C	2.55	0.48
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
2:B:99:VAL:HG23	2:B:235:MET:HE3	1.96	0.48
3:H:74:ASP:O	3:H:75:THR:C	2.56	0.48
3:E:17:THR:HB	3:E:85:SER:HA	1.96	0.48
1:D:173:GLN:O	1:D:173:GLN:HG2	2.14	0.48
1:C:116:GLN:CG	1:C:188:HIS:HD2	2.27	0.48
1:C:173:GLN:HG2	1:C:173:GLN:O	2.13	0.48
2:A:99:VAL:HG23	2:A:235:MET:HE3	1.95	0.47
3:H:17:THR:HB	3:H:85:SER:HA	1.96	0.47
3:H:65:LEU:O	3:H:67:SER:N	2.47	0.47
1:D:145:TYR:O	1:D:164:SER:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:15:ASP:N	2:A:18:THR:O	2.28	0.47
3:H:32:GLY:HA2	3:H:55:LYS:NZ	2.30	0.47
1:D:103:ASN:ND2	1:D:225:PRO:HA	2.29	0.47
4:L:115:VAL:HB	4:L:207:LYS:HG3	1.97	0.47
4:L:186:TYR:HA	4:L:192:TYR:OH	2.15	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
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
3:H:77:LYS:NZ	3:E:119:SER:O	2.37	0.45
1:D:114:ASP:HB3	1:D:265:THR:HB	1.99	0.45
2:A:14:LEU:CD2	2:A:19:LYS:HD3	2.44	0.45
1:C:112:HIS:HB2	1:C:267:THR:HB	1.98	0.45
1:D:176:TYR:CE2	1:D:195:ALA:HB2	2.52	0.45
1:C:291:ASP:OD1	1:C:292:GLY:N	2.49	0.45
1:D:112:HIS:HB2	1:D:267:THR:HB	1.98	0.45
1:C:246:GLU:OE1	2:A:105:LYS:HE2	2.17	0.45
2:A:211:ASP:OD1	3:H:58:SER:OG	2.35	0.45
3:H:152:PRO:HB2	3:H:153:GLU:O	2.17	0.44
4:F:108:ARG:HG3	4:F:171:SER:HB2	1.99	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
2:A:99:VAL:CG2	2:A:235:MET:HE3	2.47	0.44
3:H:89:ALA:O	3:H:92:THR:HG22	2.17	0.44
2:A:45:GLU:HB2	2:A:46:PRO:CD	2.48	0.44
2:A:183:THR:CG2	2:A:185:GLN:H	2.31	0.44
4:L:89:GLN:HE22	4:L:91:GLN:HG2	1.81	0.44
3:E:89:ALA:O	3:E:92:THR:HG22	2.17	0.44
1:C:240:ARG:HH21	2:A:171:GLU:CD	2.26	0.44
4:L:108:ARG:HG3	4:L:171:SER:HB2	1.99	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
3:E:105:TYR:HA	4:F:91:GLN:NE2	2.32	0.44
1:D:169:ILE:HD13	1:D:248:LEU:HD12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:185:ASN:CB	1:D:187:TRP:H	2.24	0.43
2:B:99:VAL:CG2	2:B:235:MET:HE3	2.48	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
4:L:9:SER:O	4:L:102:THR:HA	2.19	0.42
3:E:206:LYS:HB2	3:E:207:PRO:HD3	2.01	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
4:L:105:GLU:HG2	4:L:166:GLN:OE1	2.20	0.42
3:E:152:PRO:HB2	3:E:153:GLU:O	2.19	0.42
1:C:298:THR:HB	1:C:312:ASP:HB3	2.02	0.42
1:D:291:ASP:OD1	1:D:292:GLY:N	2.53	0.42
2:A:80:TRP:HB2	2:A:81:PRO:HD2	2.02	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
1:D:194:ILE:HG22	1:D:195:ALA:O	2.20	0.41
2:B:150:GLN:N	2:B:151:PRO:CD	2.82	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
1:C:77:ASN:HB2	1:C:253:ASN:HB3	2.02	0.41
2:A:267:PHE:CE1	4:L:50:ALA:HB2	2.56	0.41
4:L:159:SER:HA	4:L:178:THR:O	2.20	0.41
1:D:84:GLN:HA	1:D:245:PRO:O	2.20	0.41
1:C:185:ASN:CB	1:C:187:TRP:H	2.25	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
1:D:219:ILE:HD12	1:D:219:ILE:O	2.21	0.40
2:A:13:ASN:O	2:A:14:LEU:HG	2.22	0.40
1:D:240:ARG:HH21	2:B:171:GLU:CD	2.26	0.40
3:H:60:TYR:CD1	3:H:60:TYR:C	2.99	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:104:HIS:HB3	3:H:105:TYR:CD2	2.57	0.40
4:F:89:GLN:NE2	4:F:91:GLN:HG2	2.36	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%)	18	35
2	B	289/311 (93%)	269 (93%)	18 (6%)	2 (1%)	18	35
3	E	206/227 (91%)	190 (92%)	11 (5%)	5 (2%)	4	10
3	H	208/227 (92%)	189 (91%)	10 (5%)	9 (4%)	2	3
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%)	14	27

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	241 (93%)	17 (7%)	15	32
1	D	257/297 (86%)	241 (94%)	16 (6%)	16	34
2	A	266/283 (94%)	245 (92%)	21 (8%)	11	25
2	B	266/283 (94%)	246 (92%)	20 (8%)	12	27
3	E	180/197 (91%)	155 (86%)	25 (14%)	3	7
3	H	183/197 (93%)	158 (86%)	25 (14%)	3	7
4	F	186/188 (99%)	169 (91%)	17 (9%)	9	20
4	L	186/188 (99%)	169 (91%)	17 (9%)	9	20
All	All	1782/1930 (92%)	1624 (91%)	158 (9%)	9	20

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	47	THR
1	D	138	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	240	ARG
1	D	248	LEU
1	D	259	LYS
1	D	313	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	100	THR
2	B	126	SER
2	B	132	LEU
2	B	136	ILE
2	B	146	ILE
2	B	183	THR
2	B	185	GLN
2	B	193	ARG
2	B	225	GLU
2	B	235	MET
2	B	277	VAL
2	B	297	VAL
1	C	42	LYS
1	C	43	ASN
1	C	47	THR
1	C	138	LYS
1	C	141	SER
1	C	142	THR
1	C	154	THR
1	C	166	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	167	LYS
1	C	169	ILE
1	C	183	LYS
1	C	186	ASN
1	C	204	VAL
1	C	240	ARG
1	C	248	LEU
1	C	259	LYS
1	C	313	LYS
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	60	THR
2	A	69	ASP
2	A	100	THR
2	A	126	SER
2	A	132	LEU
2	A	136	ILE
2	A	139	GLU
2	A	146	ILE
2	A	183	THR
2	A	185	GLN
2	A	193	ARG
2	A	225	GLU
2	A	235	MET
2	A	277	VAL
2	A	297	VAL
3	H	3	GLN
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	71	ILE
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	111	LYS
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	200	ILE
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	104	VAL
4	L	136	LEU
4	L	158	ASN
4	L	180	THR
4	L	195	GLU
4	L	197	THR
4	L	205	VAL
3	E	3	GLN
3	E	14	PRO
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	67	SER
3	E	69	VAL
3	E	71	ILE
3	E	72	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	73	VAL
3	E	87	VAL
3	E	111	LYS
3	E	114	THR
3	E	116	THR
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	200	ILE
3	E	211	LYS
4	F	1	ASP
4	F	9	SER
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	104	VAL
4	F	136	LEU
4	F	158	ASN
4	F	180	THR
4	F	195	GLU
4	F	197	THR
4	F	205	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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	173	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	228	ASN
1	C	43	ASN
1	C	77	ASN
1	C	188	HIS
1	C	318	ASN
2	A	89	GLN
2	A	95	ASN
2	A	141	ASN
2	A	159	GLN
2	A	173	HIS
2	A	228	ASN
3	H	5	GLN
3	H	52	ASN
3	H	160	ASN
3	H	197	GLN
3	H	204	ASN
4	L	155	GLN
3	E	5	GLN
3	E	52	ASN
3	E	160	ASN
3	E	197	GLN
3	E	204	ASN
4	F	155	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
7	PG4	A	402	-	9,9,12	0.64	0	8,8,11	0.44	0
6	PO4	A	401	-	4,4,4	0.84	0	6,6,6	0.90	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
7	PG4	A	402	-	-	1/7/7/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	402	PG4	O4-C7-C8-O5

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, 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	C	276/319 (86%)	-0.30	3 (1%) 78 73	42, 65, 93, 104	0
1	D	275/319 (86%)	-0.31	2 (0%) 84 80	36, 63, 92, 110	0
2	A	292/311 (93%)	-0.36	1 (0%) 90 89	42, 59, 90, 126	0
2	B	293/311 (94%)	-0.32	1 (0%) 90 89	37, 60, 90, 119	0
3	E	210/227 (92%)	0.29	3 (1%) 73 67	57, 100, 154, 180	0
3	H	212/227 (93%)	-0.04	1 (0%) 87 85	51, 78, 120, 150	0
4	F	212/214 (99%)	0.08	6 (2%) 55 45	52, 81, 168, 193	0
4	L	212/214 (99%)	-0.10	3 (1%) 73 67	46, 73, 111, 120	0
All	All	1982/2142 (92%)	-0.16	20 (1%) 79 75	36, 68, 135, 193	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	191	VAL	3.0
3	E	138	GLY	2.9
4	F	190	LYS	2.8
4	L	212	GLY	2.8
1	D	163	ASN	2.6
1	C	258	GLU	2.5
3	E	129	PRO	2.5
3	H	198	THR	2.5
1	C	163	ASN	2.4
2	B	131	GLY	2.3
4	L	143	GLU	2.2
4	L	144	ALA	2.2
4	F	151	ASP	2.2
1	C	156	GLY	2.2
4	F	154	LEU	2.1
3	E	143	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	184	ALA	2.0
2	A	14	LEU	2.0
1	D	156	GLY	2.0
4	F	212	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
6	PO4	A	401	5/5	0.74	0.14	81,86,111,126	0
7	PG4	A	402	10/13	0.94	0.10	59,64,69,70	0
5	CL	D	401	1/1	0.96	0.08	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.