



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:13 PM GMT

PDB ID : 1SIO
Title : Structure of Kumamolisin-As complexed with a covalently-bound inhibitor, AcIPF
Authors : Li, M.; Wlodawer, A.; Gustchina, A.; Tsuruoka, N.; Ashida, M.; Minakata, H.; Oyama, H.; Oda, K.; Nishino, T.; Nakayama, T.
Deposited on : 2004-03-01
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
<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

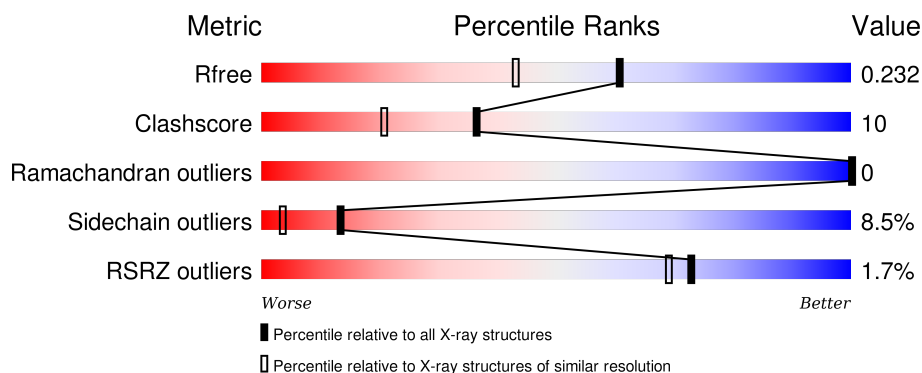
1 Overall quality at a glance

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.



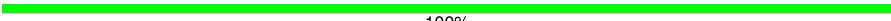
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 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 $\leq 5\%$. 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	A	364	<div> <div>81%</div> <div>14%</div> <div>...</div> </div>
1	B	364	<div> <div>74%</div> <div>22%</div> <div>..</div> </div>
1	C	364	<div> <div>4%</div> <div>70%</div> <div>23%</div> <div>.</div> </div>
2	D	4	<div> <div>100%</div> </div>
2	E	4	<div> <div>100%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	4	 100%

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	SO4	A	501	-	-	-	X
3	SO4	B	502	-	-	X	-
3	SO4	C	503	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8621 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 kumamolisin-As.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	1
			2537	1598	425	510	4			
1	B	356	Total	C	N	O	S	0	0	1
			2532	1595	424	509	4			
1	C	353	Total	C	N	O	S	0	0	1
			2512	1581	421	506	4			

- Molecule 2 is a protein called Ace-ILE-PRO-PHL peptide inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			29	22	3	4			
2	E	4	Total	C	N	O	0	0	0
			29	22	3	4			
2	F	4	Total	C	N	O	0	0	0
			29	22	3	4			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	375	Total	O	0	0
			375	375		
5	D	7	Total	O	0	0
			7	7		
5	B	354	Total	O	0	0
			354	354		

Continued on next page...

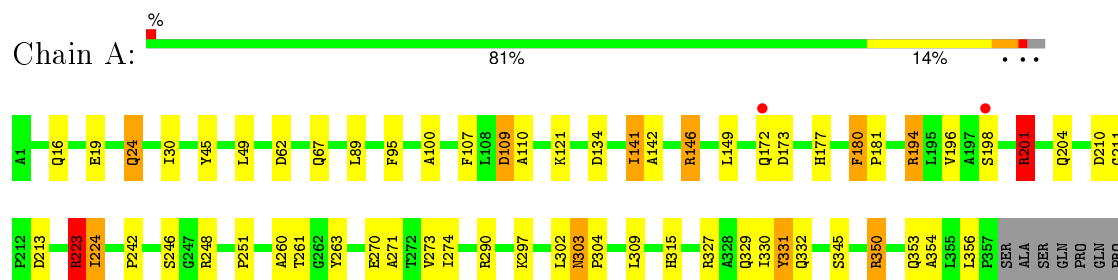
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	196	Total 196	O 196	0	0
5	E	1	Total 1	O 1	0	0
5	F	2	Total 2	O 2	0	0

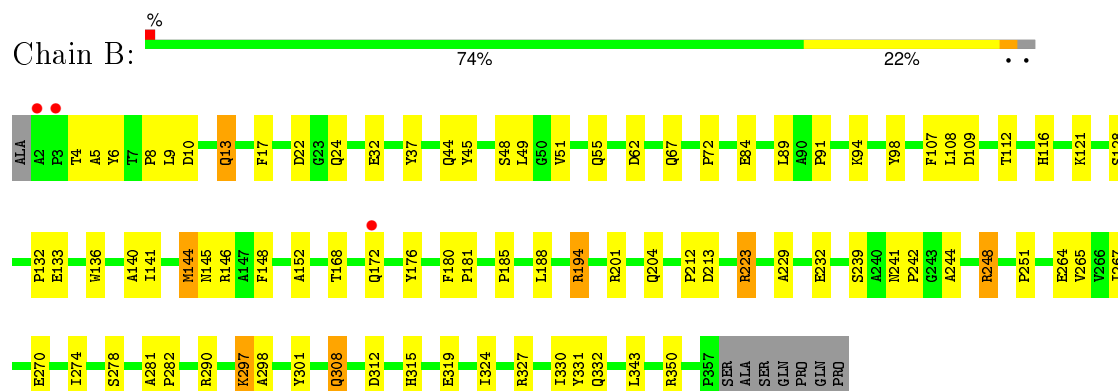
3 Residue-property plots

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.

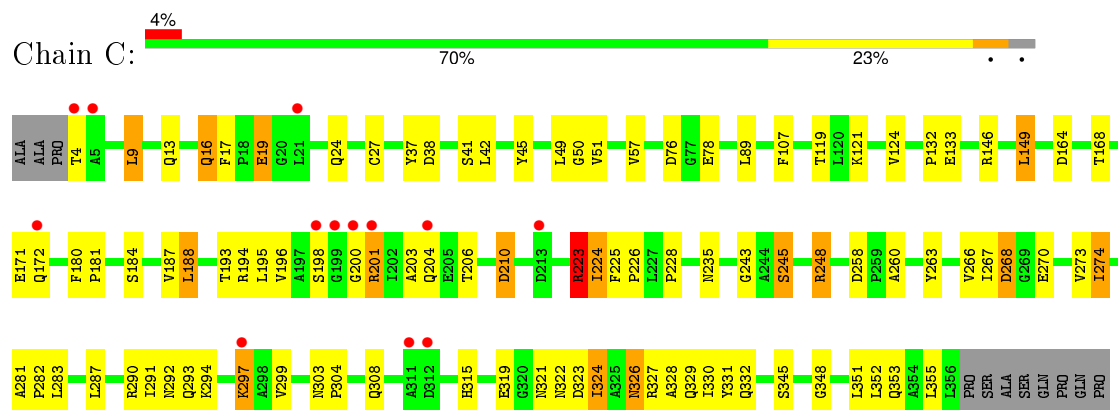
- Molecule 1: kumamolisin-As



- Molecule 1: kumamolisin-As



- Molecule 1: kumamolisin-As



- Molecule 2: Ace-ILE-PRO-PHL peptide inhibitor

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Ace-ILE-PRO-PHL peptide inhibitor

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Ace-ILE-PRO-PHL peptide inhibitor

Chain F:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.37Å 238.73Å 49.25Å 90.00° 113.70° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 24.90 – 1.80	Depositor EDS
% Data completeness (in resolution range)	88.2 (10.00-1.80) 92.6 (24.90-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 1.80Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.173 , 0.243 0.167 , 0.232	Depositor DCC
R_{free} test set	4457 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.4	EDS
Estimated twinning fraction	0.036 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 89192 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8621	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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, 0.375 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: CA, SO4, ACE, PHL

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	0.64	0/2600	1.48	22/3573 (0.6%)
1	B	0.60	0/2595	1.45	23/3566 (0.6%)
1	C	0.55	0/2574	1.39	18/3536 (0.5%)
2	D	0.65	0/16	1.33	0/22
2	E	0.50	0/16	1.33	0/22
2	F	0.50	0/16	1.36	0/22
All	All	0.60	0/7817	1.44	63/10741 (0.6%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	ARG	NE-CZ-NH1	13.55	127.07	120.30
1	B	223	ARG	NE-CZ-NH2	-12.44	114.08	120.30
1	A	327	ARG	CD-NE-CZ	11.22	139.31	123.60
1	C	45	TYR	CB-CG-CD2	11.19	127.71	121.00
1	A	350	ARG	NE-CZ-NH2	-10.93	114.83	120.30
1	C	223	ARG	NE-CZ-NH1	10.47	125.54	120.30
1	B	194	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	B	194	ARG	CD-NE-CZ	9.45	136.83	123.60
1	C	223	ARG	CD-NE-CZ	9.13	136.38	123.60
1	A	290	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	C	45	TYR	CB-CG-CD1	-8.26	116.04	121.00
1	B	37	TYR	CB-CG-CD1	8.24	125.94	121.00
1	B	248	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	B	248	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	B	350	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	B	301	TYR	CB-CG-CD2	-7.55	116.47	121.00
1	B	301	TYR	CB-CG-CD1	7.43	125.46	121.00
1	B	223	ARG	NE-CZ-NH1	7.40	124.00	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	ARG	NE-CZ-NH1	-7.39	116.61	120.30
1	A	223	ARG	CD-NE-CZ	7.23	133.72	123.60
1	B	223	ARG	CD-NE-CZ	7.06	133.48	123.60
1	A	95	PHE	CB-CG-CD2	-6.90	115.97	120.80
1	B	343	LEU	C-N-CA	6.81	136.59	122.30
1	C	248	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	B	290	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	C	263	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	C	263	TYR	CB-CG-CD1	6.55	124.93	121.00
1	A	331	TYR	CD1-CE1-CZ	-6.53	113.92	119.80
1	B	176	TYR	CG-CD1-CE1	-6.43	116.16	121.30
1	A	223	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	B	13	GLN	CB-CG-CD	6.35	128.11	111.60
1	A	331	TYR	CG-CD2-CE2	-6.17	116.36	121.30
1	A	201	ARG	CD-NE-CZ	6.10	132.14	123.60
1	C	210	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	261	THR	C-N-CA	6.05	135.01	122.30
1	B	176	TYR	CA-CB-CG	-6.00	102.00	113.40
1	A	211	GLY	CA-C-O	5.96	131.34	120.60
1	C	248	ARG	C-N-CA	-5.89	109.93	122.30
1	B	98	TYR	CB-CG-CD2	5.86	124.51	121.00
1	C	78	GLU	CG-CD-OE2	5.77	129.84	118.30
1	A	180	PHE	CB-CG-CD1	-5.63	116.86	120.80
1	B	148	PHE	CB-CG-CD1	5.57	124.70	120.80
1	A	303	ASN	O-C-N	5.50	131.55	121.10
1	B	32	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	A	327	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	37	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	C	27	CYS	O-C-N	5.40	131.35	122.70
1	A	274	ILE	O-C-N	5.38	132.34	123.20
1	A	109	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	98	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	A	201	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	45	TYR	CA-CB-CG	-5.31	103.31	113.40
1	C	164	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	C	223	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	319	GLU	C-N-CA	5.15	133.12	122.30
1	C	188	LEU	CA-CB-CG	5.12	127.07	115.30
1	B	17	PHE	CG-CD1-CE1	-5.10	115.19	120.80
1	C	164	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	37	TYR	CB-CG-CD1	5.09	124.05	121.00
1	A	45	TYR	CB-CG-CD1	-5.08	117.95	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	210	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	C	268	ASP	C-N-CA	5.00	132.81	122.30

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	2537	0	2427	37	0
1	B	2532	0	2419	50	0
1	C	2512	0	2396	59	0
2	D	29	0	31	0	0
2	E	29	0	31	0	0
2	F	29	0	31	0	0
3	A	5	0	0	1	0
3	B	5	0	0	2	0
3	C	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	375	0	0	13	0
5	B	354	0	0	15	0
5	C	196	0	0	16	0
5	D	7	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
All	All	8621	0	7335	143	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 10.

All (143) 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:C:196:VAL:HG12	1:C:203:ALA:HB3	1.46	0.97
1:C:9:LEU:HD11	1:C:49:LEU:HD22	1.49	0.93
1:A:223:ARG:HG2	1:A:223:ARG:HH11	1.41	0.85
1:C:196:VAL:HB	1:C:204:GLN:HG3	1.66	0.78
1:C:146:ARG:HD2	1:C:149:LEU:HD12	1.66	0.77
1:C:198:SER:O	1:C:201:ARG:HG3	1.85	0.77
1:C:171:GLU:HG3	5:C:2190:HOH:O	1.83	0.77
1:C:223:ARG:HH11	1:C:223:ARG:HB2	1.50	0.76
1:A:24:GLN:HG3	5:A:1878:HOH:O	1.86	0.75
1:B:152:ALA:HB2	5:B:2182:HOH:O	1.86	0.75
1:C:273:VAL:O	1:C:274:ILE:HD13	1.88	0.74
1:B:223:ARG:HD3	3:B:502:SO4:O1	1.87	0.73
1:C:223:ARG:HD3	5:C:2220:HOH:O	1.90	0.71
1:C:321:ASN:HB2	5:C:2013:HOH:O	1.90	0.70
1:B:308:GLN:HB3	5:B:1852:HOH:O	1.91	0.68
1:B:13:GLN:HB2	5:B:2116:HOH:O	1.96	0.66
1:C:245:SER:HB3	5:C:2014:HOH:O	1.94	0.66
1:A:149:LEU:HD11	1:C:50:GLY:HA2	1.79	0.65
1:A:67:GLN:HG3	5:A:2081:HOH:O	1.97	0.65
1:C:294:LYS:HG2	1:C:352:LEU:HD21	1.80	0.63
1:C:4:THR:HG21	5:C:1953:HOH:O	1.97	0.63
1:A:196:VAL:HB	1:A:204:GLN:HG2	1.80	0.62
1:C:324:ILE:HA	5:C:2092:HOH:O	2.02	0.60
1:B:48:SER:HB2	5:B:2123:HOH:O	2.02	0.59
1:B:229:ALA:O	1:B:232:GLU:HG2	2.03	0.58
1:B:72:PRO:HA	1:B:267:ILE:HG22	1.85	0.58
1:A:353:GLN:OE1	1:A:356:LEU:HD12	2.04	0.57
1:A:315:HIS:HD2	5:A:1615:HOH:O	1.87	0.56
1:C:266:VAL:O	1:C:267:ILE:HD13	2.05	0.56
1:C:292:ASN:OD1	1:C:299:VAL:HG22	2.06	0.56
1:C:326:ASN:HD22	1:C:328:ALA:H	1.53	0.55
1:C:196:VAL:HA	5:C:1933:HOH:O	2.07	0.54
1:B:239:SER:HB3	1:B:244:ALA:CB	2.37	0.54
1:B:6:TYR:HB3	1:B:10:ASP:HB2	1.89	0.54
1:A:146:ARG:HH11	1:A:146:ARG:HG3	1.72	0.54
1:A:270:GLU:HG3	5:A:1815:HOH:O	2.06	0.54
1:B:194:ARG:HD3	5:B:1661:HOH:O	2.08	0.54
1:C:119:THR:HG21	5:C:2390:HOH:O	2.08	0.53
1:B:49:LEU:HB3	1:B:51:VAL:HG13	1.89	0.53
1:A:198:SER:O	1:A:201:ARG:HG3	2.08	0.53
1:B:146:ARG:HG3	5:B:2374:HOH:O	2.09	0.52
1:C:89:LEU:CD2	1:C:283:LEU:HD12	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PHE:CG	1:A:181:PRO:HA	2.44	0.51
1:C:351:LEU:O	1:C:355:LEU:HG	2.10	0.51
1:A:315:HIS:HB3	1:A:345:SER:OG	2.09	0.51
1:C:194:ARG:HD2	1:C:258:ASP:OD2	2.11	0.51
1:B:297:LYS:HG2	1:B:298:ALA:N	2.26	0.51
1:B:116:HIS:HE1	5:B:1679:HOH:O	1.94	0.51
1:A:271:ALA:HB1	1:B:201:ARG:CZ	2.41	0.50
1:A:329:GLN:HG2	5:A:2169:HOH:O	2.12	0.50
5:A:1943:HOH:O	1:B:315:HIS:HD2	1.95	0.50
1:A:223:ARG:HG2	1:A:223:ARG:NH1	2.16	0.49
1:B:133:GLU:OE2	3:B:502:SO4:O4	2.30	0.49
1:B:44:GLN:O	1:B:48:SER:OG	2.29	0.49
1:A:142:ALA:O	1:A:146:ARG:HD3	2.12	0.49
1:B:108:LEU:O	1:B:112:THR:HG23	2.11	0.49
1:A:303:ASN:HB2	1:A:304:PRO:HD3	1.94	0.49
1:C:180:PHE:CG	1:C:181:PRO:HA	2.47	0.49
1:B:128:SER:HB3	1:B:278:SER:HA	1.94	0.49
1:C:76:ASP:OD2	1:C:268:ASP:OD2	2.30	0.49
1:B:9:LEU:HD12	1:B:49:LEU:HD22	1.95	0.49
1:C:17:PHE:CZ	1:C:287:LEU:HB2	2.47	0.49
1:A:100:ALA:HB2	1:A:110:ALA:HB2	1.95	0.49
1:C:201:ARG:HH11	1:C:201:ARG:HG2	1.78	0.49
1:C:180:PHE:CD1	1:C:181:PRO:HA	2.49	0.48
1:B:212:PRO:HG3	1:B:324:ILE:O	2.14	0.48
1:C:329:GLN:O	1:C:332:GLN:HG3	2.14	0.48
1:C:132:PRO:HG3	5:C:2190:HOH:O	2.13	0.48
1:B:264:GLU:HB3	5:B:1874:HOH:O	2.14	0.47
1:C:291:ILE:HG21	1:C:355:LEU:HD12	1.97	0.47
1:B:241:ASN:HA	1:B:242:PRO:HD3	1.77	0.47
1:A:330:ILE:HA	1:A:331:TYR:HA	1.65	0.47
1:C:16:GLN:O	1:C:348:GLY:HA3	2.15	0.47
1:B:265:VAL:HG21	1:B:274:ILE:HD12	1.97	0.47
1:A:121:LYS:HB2	1:A:121:LYS:HE2	1.58	0.47
1:C:9:LEU:CD1	1:C:49:LEU:HD22	2.35	0.46
1:A:350:ARG:NE	5:A:1519:HOH:O	2.48	0.46
1:C:210:ASP:OD2	1:C:258:ASP:OD1	2.33	0.46
1:B:132:PRO:O	1:B:136:TRP:HD1	1.98	0.46
1:B:145:ASN:HD21	1:B:185:PRO:HD2	1.81	0.46
1:C:294:LYS:HD2	1:C:294:LYS:HA	1.74	0.46
1:C:19:GLU:OE1	1:C:19:GLU:HA	2.16	0.46
1:C:243:GLY:HA3	5:C:2314:HOH:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ASN:HB2	1:C:304:PRO:HD3	1.98	0.46
1:A:146:ARG:NH1	1:A:146:ARG:HG3	2.28	0.46
1:C:4:THR:N	1:C:260:ALA:O	2.49	0.46
1:B:136:TRP:HB2	1:B:141:ILE:HD11	1.98	0.46
1:A:260:ALA:HB2	1:B:312:ASP:HB3	1.98	0.46
1:B:194:ARG:NH1	5:B:2408:HOH:O	2.49	0.45
1:C:323:ASP:N	5:C:2013:HOH:O	2.49	0.45
1:C:13:GLN:NE2	5:C:2113:HOH:O	2.49	0.45
1:B:315:HIS:HE1	5:B:2138:HOH:O	2.00	0.45
1:A:350:ARG:NH2	5:A:1989:HOH:O	2.49	0.45
1:B:140:ALA:HB1	5:B:1969:HOH:O	2.16	0.45
1:B:55:GLN:HE22	1:B:94:LYS:HE2	1.82	0.45
1:B:180:PHE:CG	1:B:181:PRO:HA	2.52	0.45
1:B:297:LYS:NZ	5:B:2360:HOH:O	2.50	0.44
1:B:8:PRO:HG2	1:B:45:TYR:OH	2.17	0.44
1:B:330:ILE:HA	1:B:331:TYR:HA	1.85	0.44
1:C:322:ASN:N	5:C:2013:HOH:O	2.49	0.44
1:B:45:TYR:CE2	1:B:84:GLU:HB3	2.52	0.44
1:C:281:ALA:HB3	1:C:282:PRO:HD3	2.00	0.44
1:B:22:ASP:HB2	1:B:91:PRO:HG2	1.99	0.44
1:A:173:ASP:CG	1:A:177:HIS:HE2	2.21	0.44
1:B:239:SER:HB3	1:B:244:ALA:HB3	2.00	0.44
1:A:194:ARG:NH1	5:A:2101:HOH:O	2.49	0.44
1:A:146:ARG:NH1	5:A:1925:HOH:O	2.50	0.44
1:C:291:ILE:HD13	1:C:355:LEU:HD12	1.99	0.44
1:C:194:ARG:NH1	5:C:1963:HOH:O	2.50	0.44
1:B:213:ASP:HB2	5:B:2065:HOH:O	2.17	0.44
1:B:121:LYS:NZ	5:B:2115:HOH:O	2.50	0.44
1:C:297:LYS:HE3	1:C:297:LYS:HB3	1.91	0.44
1:C:223:ARG:NH1	5:C:1801:HOH:O	2.50	0.43
1:C:225:PHE:HA	1:C:226:PRO:HD3	1.81	0.43
1:A:146:ARG:NH1	5:A:2119:HOH:O	2.50	0.43
1:A:194:ARG:NH2	5:A:1549:HOH:O	2.49	0.43
1:A:16:GLN:NE2	5:A:1887:HOH:O	2.50	0.43
1:B:297:LYS:HE3	1:B:297:LYS:HB3	1.14	0.43
1:C:290:ARG:O	1:C:293:GLN:HB3	2.18	0.43
1:C:224:ILE:HD13	1:C:224:ILE:N	2.34	0.43
1:C:228:PRO:HA	5:C:2253:HOH:O	2.18	0.43
1:B:5:ALA:HB1	1:B:264:GLU:HG3	2.01	0.42
1:A:309:LEU:HD22	1:A:354:ALA:HB1	2.01	0.42
1:A:62:ASP:OD2	1:A:109:ASP:OD2	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:LYS:O	1:C:297:LYS:HG2	2.18	0.42
1:B:229:ALA:HA	1:B:232:GLU:HG2	2.02	0.42
1:A:224:ILE:N	1:A:224:ILE:HD13	2.34	0.42
1:B:204:GLN:HG3	5:B:2202:HOH:O	2.18	0.42
1:C:193:THR:HB	1:C:206:THR:O	2.19	0.42
1:A:30:ILE:HD13	1:A:30:ILE:HG21	1.80	0.42
1:B:144:MET:HE3	1:B:144:MET:HB3	1.99	0.41
1:B:281:ALA:HB3	1:B:282:PRO:HD3	2.02	0.41
1:A:19:GLU:HG2	3:A:501:SO4:O1	2.20	0.41
1:A:141:ILE:HG21	1:A:141:ILE:HD12	1.84	0.41
1:A:263:TYR:O	1:A:273:VAL:HA	2.21	0.41
1:C:184:SER:HB3	1:C:187:VAL:CG2	2.51	0.41
1:C:38:ASP:OD1	1:C:41:SER:OG	2.29	0.41
1:C:195:LEU:HD12	1:C:196:VAL:N	2.36	0.40
1:C:330:ILE:HA	1:C:331:TYR:HA	1.92	0.40
1:B:239:SER:HB3	1:B:244:ALA:HB1	2.03	0.40
1:B:62:ASP:OD2	1:B:109:ASP:OD2	2.40	0.40
1:C:315:HIS:HB3	1:C:345:SER:OG	2.22	0.40
1:C:13:GLN:NE2	1:C:200:GLY:HA2	2.37	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	355/364 (98%)	349 (98%)	6 (2%)	0	100	100
1	B	354/364 (97%)	346 (98%)	8 (2%)	0	100	100
1	C	351/364 (96%)	336 (96%)	15 (4%)	0	100	100
2	D	2/4 (50%)	2 (100%)	0	0	100	100
2	E	2/4 (50%)	2 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1066/1104 (97%)	1037 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	253/260 (97%)	233 (92%)	20 (8%)	15	4
1	B	253/260 (97%)	237 (94%)	16 (6%)	22	8
1	C	251/260 (96%)	222 (88%)	29 (12%)	7	1
2	D	2/2 (100%)	2 (100%)	0	100	100
2	E	2/2 (100%)	2 (100%)	0	100	100
2	F	2/2 (100%)	2 (100%)	0	100	100
All	All	763/786 (97%)	698 (92%)	65 (8%)	13	3

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	49	LEU
1	A	89	LEU
1	A	107	PHE
1	A	134	ASP
1	A	141	ILE
1	A	146	ARG
1	A	172	GLN
1	A	194	ARG
1	A	201	ARG
1	A	213	ASP
1	A	223	ARG
1	A	224	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	242	PRO
1	A	246	SER
1	A	248	ARG
1	A	251	PRO
1	A	297	LYS
1	A	302	LEU
1	A	332	GLN
1	B	4	THR
1	B	24	GLN
1	B	67	GLN
1	B	89	LEU
1	B	107	PHE
1	B	144	MET
1	B	168	THR
1	B	172	GLN
1	B	188	LEU
1	B	248	ARG
1	B	251	PRO
1	B	270	GLU
1	B	297	LYS
1	B	308	GLN
1	B	319	GLU
1	B	332	GLN
1	C	9	LEU
1	C	16	GLN
1	C	19	GLU
1	C	24	GLN
1	C	42	LEU
1	C	51	VAL
1	C	57	VAL
1	C	107	PHE
1	C	121	LYS
1	C	124	VAL
1	C	133	GLU
1	C	149	LEU
1	C	168	THR
1	C	172	GLN
1	C	188	LEU
1	C	201	ARG
1	C	223	ARG
1	C	224	ILE
1	C	235	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	245	SER
1	C	248	ARG
1	C	270	GLU
1	C	274	ILE
1	C	297	LYS
1	C	308	GLN
1	C	324	ILE
1	C	326	ASN
1	C	327	ARG
1	C	353	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	16	GLN
1	A	24	GLN
1	A	44	GLN
1	A	55	GLN
1	A	145	ASN
1	A	172	GLN
1	A	303	ASN
1	A	315	HIS
1	B	13	GLN
1	B	44	GLN
1	B	55	GLN
1	B	116	HIS
1	B	145	ASN
1	B	204	GLN
1	B	315	HIS
1	B	329	GLN
1	C	13	GLN
1	C	16	GLN
1	C	24	GLN
1	C	55	GLN
1	C	145	ASN
1	C	326	ASN
1	C	329	GLN
1	C	332	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
2	PHL	D	4	1,2	11,11,11	0.56	0	10,13,13	0.64	0
2	PHL	E	4	1,2	11,11,11	0.49	0	10,13,13	0.75	0
2	PHL	F	4	1,2	11,11,11	0.51	0	10,13,13	0.67	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
2	PHL	D	4	1,2	-	0/6/6/6	0/1/1/1
2	PHL	E	4	1,2	-	0/6/6/6	0/1/1/1
2	PHL	F	4	1,2	-	0/6/6/6	0/1/1/1

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.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	SO4	A	501	-	4,4,4	1.02	0	6,6,6	0.37	0
3	SO4	B	502	-	4,4,4	1.01	0	6,6,6	0.50	0
3	SO4	C	503	-	4,4,4	1.07	0	6,6,6	0.39	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
3	SO4	A	501	-	-	0/0/0/0	0/0/0/0
3	SO4	B	502	-	-	0/0/0/0	0/0/0/0
3	SO4	C	503	-	-	0/0/0/0	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	SO4	1	0
3	B	502	SO4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	357/364 (98%)	-0.39	2 (0%) 90 88	11, 18, 35, 60	0
1	B	356/364 (97%)	-0.39	3 (0%) 87 85	11, 19, 36, 63	0
1	C	353/364 (96%)	0.10	13 (3%) 45 39	13, 28, 54, 82	0
2	D	2/4 (50%)	-0.69	0 100 100	15, 15, 15, 21	0
2	E	2/4 (50%)	-1.01	0 100 100	18, 18, 18, 19	0
2	F	2/4 (50%)	-0.82	0 100 100	20, 20, 20, 24	0
All	All	1072/1104 (97%)	-0.23	18 (1%) 73 69	11, 21, 43, 82	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	201	ARG	4.6
1	B	3	PRO	4.6
1	C	199	GLY	4.1
1	C	198	SER	3.9
1	C	4	THR	3.2
1	B	2	ALA	2.8
1	C	200	GLY	2.7
1	C	5	ALA	2.7
1	C	172	GLN	2.6
1	C	21	LEU	2.4
1	C	213	ASP	2.2
1	C	204	GLN	2.2
1	C	312	ASP	2.1
1	A	198	SER	2.1
1	C	311	ALA	2.1
1	B	172	GLN	2.1
1	C	297	LYS	2.0
1	A	172	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	PHL	F	4	11/11	0.96	0.07	-	18,22,27,28	0
2	PHL	D	4	11/11	0.96	0.08	-	7,14,20,23	0
2	PHL	E	4	11/11	0.95	0.07	-	9,16,18,20	0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	C	503	5/5	0.89	0.23	5.61	41,68,70,103	0
3	SO4	A	501	5/5	0.93	0.17	4.58	30,46,58,68	0
3	SO4	B	502	5/5	0.97	0.09	1.23	32,33,37,38	0
4	CA	B	602	1/1	1.00	0.07	-0.81	18,18,18,18	0
4	CA	C	603	1/1	0.97	0.05	-1.69	41,41,41,41	0
4	CA	A	601	1/1	0.99	0.05	-2.16	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.