



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:32 PM UTC

PDB ID : 1SIO / pdb_00001sio
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

<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

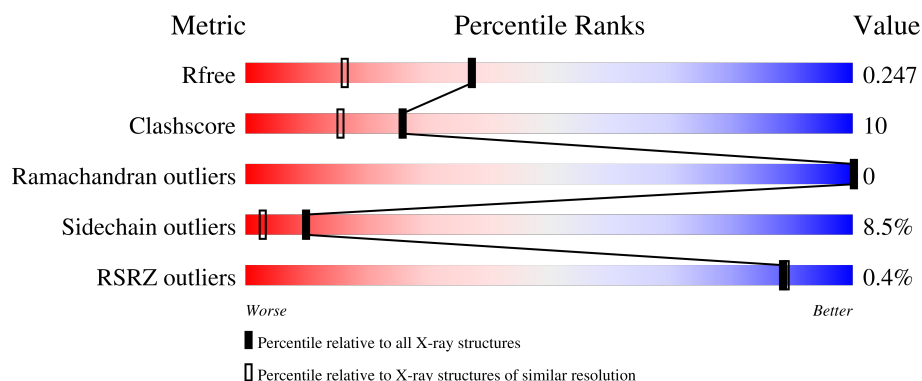
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

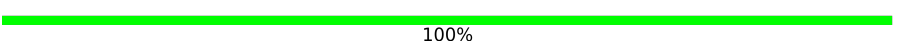
The reported resolution of this entry is 1.80 Å.

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 75% 18% 7% 0% 0%
1	B	364	 70% 24% 7% 0% 0%
1	C	364	 63% 26% 7% 0% 0%
2	D	4	 100%
2	E	4	 75% 25%

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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	B	502	-	-	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 (CCD ID: 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 (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	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	B	354	Total	O	0	0
			354	354		
5	C	196	Total	O	0	0
			196	196		

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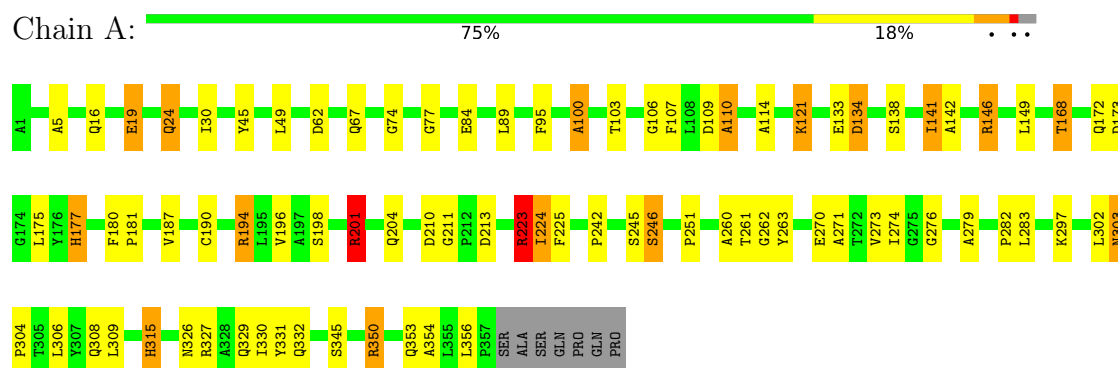
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	7	Total	O	0	0
			7	7		
5	E	1	Total	O	0	0
			1	1		
5	F	2	Total	O	0	0
			2	2		

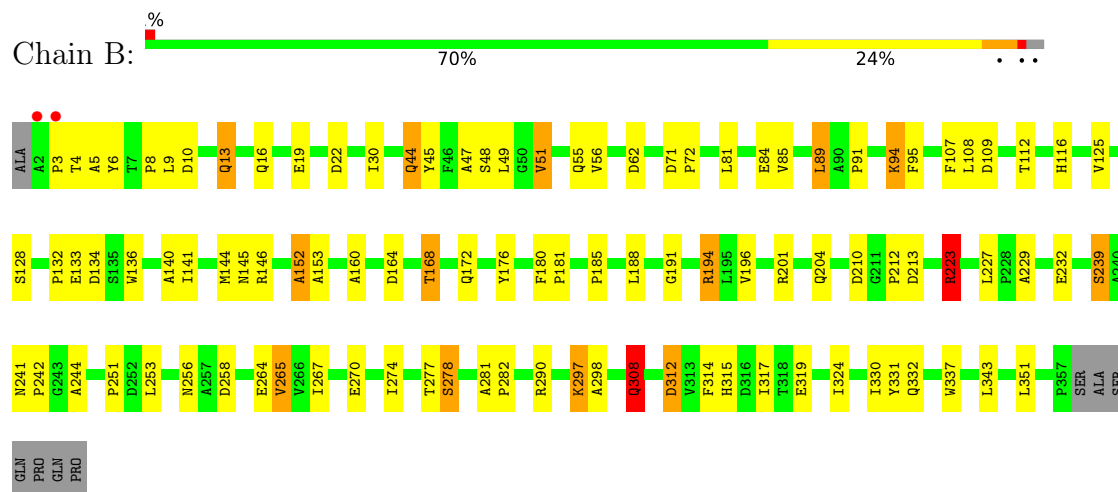
3 Residue-property plots [i](#)

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.

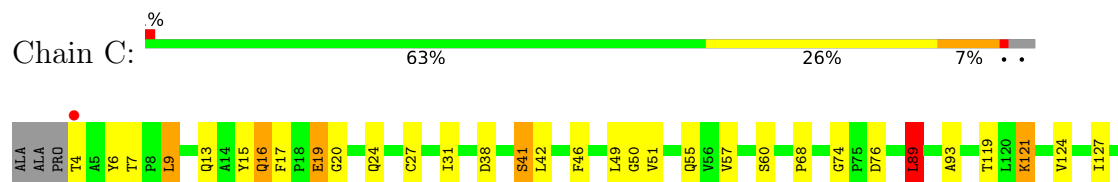
• Molecule 1: kumamolisin-As

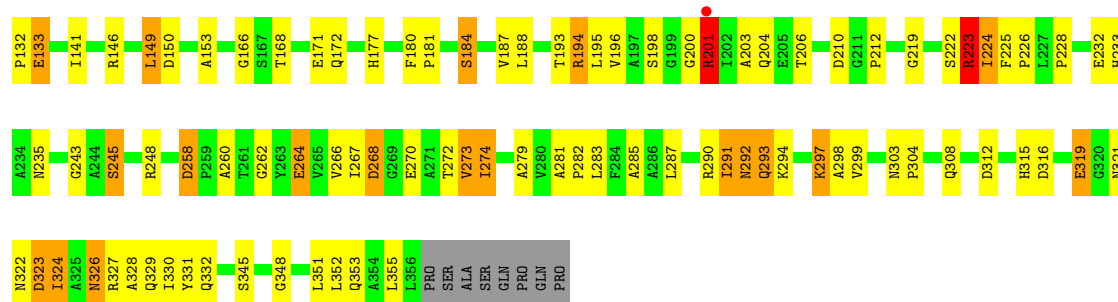


• Molecule 1: kumamolisin-As



• 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: 75% 25%



- 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 10.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	88.2 (10.00-1.80) 92.3 (10.00-1.80)	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 0.184 , 0.247	Depositor DCC
R_{free} test set	4478 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for l,-k,h	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, 0.333 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: PHL, ACE, SO4, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.83	0/2600	1.88	53/3573 (1.5%)
1	B	0.76	0/2595	1.85	57/3566 (1.6%)
1	C	0.71	1/2574 (0.0%)	1.89	64/3536 (1.8%)
2	D	0.84	0/16	1.34	0/22
2	E	0.63	0/16	1.50	1/22 (4.5%)
2	F	0.58	0/16	1.44	0/22
All	All	0.77	1/7817 (0.0%)	1.87	175/10741 (1.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	121	LYS	CA-CB	5.75	1.57	1.52

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	ASN	O-C-N	14.14	131.55	120.38
1	C	248	ARG	CA-C-N	-12.82	109.93	122.36
1	C	248	ARG	C-N-CA	-12.82	109.93	122.36
1	A	121	LYS	O-C-N	-12.63	115.72	121.53
1	C	121	LYS	O-C-N	-12.20	115.92	121.53
1	A	327	ARG	CD-NE-CZ	10.65	139.31	124.40
1	C	121	LYS	CA-C-O	10.55	128.70	120.26
1	A	261	THR	CA-C-N	9.33	135.01	121.67
1	A	261	THR	C-N-CA	9.33	135.01	121.67
1	C	212	PRO	CA-C-N	9.13	132.86	120.44
1	C	212	PRO	C-N-CA	9.13	132.86	120.44
1	A	303	ASN	CA-C-O	-9.13	110.41	119.08
1	B	13	GLN	CB-CG-CD	9.13	128.11	112.60
1	B	194	ARG	CD-NE-CZ	8.88	136.83	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	121	LYS	N-CA-CB	-8.87	101.81	111.66
1	A	95	PHE	CA-CB-CG	-8.78	105.02	113.80
1	C	223	ARG	CD-NE-CZ	8.56	136.38	124.40
1	A	274	ILE	O-C-N	8.49	132.34	123.00
1	A	315	HIS	CA-CB-CG	-8.46	105.34	113.80
1	B	16	GLN	OE1-CD-NE2	-8.15	114.45	122.60
1	C	7	THR	N-CA-CB	8.07	118.92	109.72
1	C	279	ALA	CA-C-O	7.92	128.54	119.27
1	B	85	VAL	O-C-N	7.79	130.00	121.90
1	B	343	LEU	CA-C-N	7.75	136.59	121.41
1	B	343	LEU	C-N-CA	7.75	136.59	121.41
1	B	30	ILE	CA-C-O	-7.66	112.53	120.27
1	C	7	THR	CA-C-O	-7.63	113.34	121.27
1	B	164	ASP	CA-CB-CG	7.55	120.15	112.60
1	B	107	PHE	CA-CB-CG	7.53	121.33	113.80
1	C	316	ASP	O-C-N	-7.30	114.73	123.13
1	C	264	GLU	CA-C-N	7.23	132.87	123.03
1	C	264	GLU	C-N-CA	7.23	132.87	123.03
1	A	306	LEU	CA-C-O	7.15	128.35	120.63
1	A	134	ASP	CA-CB-CG	6.98	119.58	112.60
1	A	210	ASP	CA-C-O	6.96	128.97	120.55
1	C	27	CYS	O-C-N	6.87	131.35	123.31
1	A	211	GLY	CA-C-O	6.86	131.34	121.52
1	B	125	VAL	CA-C-O	-6.81	113.24	120.39
1	A	74	GLY	O-C-N	6.78	128.55	121.77
1	C	316	ASP	CA-C-O	6.74	127.98	120.43
1	A	223	ARG	CD-NE-CZ	6.66	133.72	124.40
1	B	134	ASP	CA-CB-CG	6.62	119.22	112.60
1	B	176	TYR	CA-CB-CG	-6.61	102.00	113.90
1	B	258	ASP	O-C-N	-6.55	115.61	121.31
1	B	239	SER	CA-C-O	-6.55	114.61	121.55
1	C	46	PHE	CA-CB-CG	-6.54	107.26	113.80
1	C	319	GLU	CA-C-N	6.53	133.12	122.21
1	C	319	GLU	C-N-CA	6.53	133.12	122.21
1	B	85	VAL	CA-C-O	-6.50	113.83	121.05
1	B	223	ARG	CD-NE-CZ	6.49	133.48	124.40
1	A	274	ILE	CA-C-O	-6.48	115.06	121.67
1	C	6	TYR	CA-C-N	-6.47	111.45	123.55
1	C	6	TYR	C-N-CA	-6.47	111.45	123.55
1	A	24	GLN	OE1-CD-NE2	6.46	129.06	122.60
1	B	196	VAL	O-C-N	6.42	129.85	122.99
1	C	323	ASP	CA-C-O	-6.36	113.36	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	31	ILE	O-C-N	6.34	130.18	122.95
1	A	168	THR	CA-C-O	6.33	126.37	119.15
1	C	133	GLU	O-C-N	-6.33	114.99	122.20
1	B	81	LEU	CA-C-O	6.27	127.20	120.55
1	C	55	GLN	CA-C-O	-6.25	113.57	120.69
1	C	268	ASP	CA-C-N	6.23	132.81	121.85
1	C	268	ASP	C-N-CA	6.23	132.81	121.85
1	A	121	LYS	CA-C-O	6.22	125.23	120.26
1	C	166	GLY	O-C-N	6.19	128.79	122.91
1	B	337	TRP	CA-C-O	-6.18	114.39	121.19
1	A	326	ASN	CA-C-O	-6.13	114.57	121.25
1	A	225	PHE	CA-CB-CG	-6.12	107.68	113.80
1	C	177	HIS	CA-C-N	-6.07	115.78	122.27
1	C	177	HIS	C-N-CA	-6.07	115.78	122.27
1	B	71	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	107	PHE	CA-C-O	6.02	126.90	120.70
1	A	283	LEU	CA-C-O	6.00	127.12	120.82
1	B	265	VAL	CA-C-O	-5.99	115.77	121.64
1	B	95	PHE	CA-CB-CG	-5.98	107.82	113.80
1	C	7	THR	N-CA-C	-5.92	103.21	110.31
1	B	308	GLN	OE1-CD-NE2	5.89	128.50	122.60
1	A	45	TYR	CA-CB-CG	-5.89	103.31	113.90
1	C	89	LEU	CA-C-N	-5.86	116.32	122.89
1	C	89	LEU	C-N-CA	-5.86	116.32	122.89
1	C	292	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	245	SER	CA-C-N	5.81	128.96	120.71
1	A	245	SER	C-N-CA	5.81	128.96	120.71
1	A	246	SER	CA-C-O	-5.81	114.80	121.19
1	C	285	ALA	O-C-N	5.81	128.28	122.12
1	A	110	ALA	N-CA-C	-5.80	105.03	111.36
1	B	13	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	A	100	ALA	O-C-N	5.78	125.41	121.71
1	B	227	LEU	O-C-N	-5.78	116.29	121.31
1	B	277	THR	CA-C-N	5.75	128.78	120.38
1	B	277	THR	C-N-CA	5.75	128.78	120.38
1	B	56	VAL	CA-C-N	-5.75	114.95	122.94
1	B	56	VAL	C-N-CA	-5.75	114.95	122.94
1	B	314	PHE	CA-CB-CG	-5.75	108.06	113.80
1	B	160	ALA	CA-C-N	5.73	128.85	120.71
1	B	160	ALA	C-N-CA	5.73	128.85	120.71
1	C	150	ASP	CA-CB-CG	-5.73	106.87	112.60
1	A	77	GLY	N-CA-C	-5.72	105.75	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	SER	CA-C-O	-5.70	114.92	119.71
1	B	223	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	C	68	PRO	CA-C-O	-5.65	114.58	121.03
1	C	141	ILE	CA-C-O	5.63	127.14	121.17
1	A	276	GLY	N-CA-C	-5.62	104.65	112.18
1	A	175	LEU	CA-C-O	-5.61	114.77	121.11
1	A	84	GLU	O-C-N	-5.61	115.76	122.15
1	A	107	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	327	ARG	NE-CZ-NH1	5.57	127.07	121.50
1	C	74	GLY	O-C-N	5.55	127.32	121.77
1	B	168	THR	CA-C-N	5.54	130.00	122.07
1	B	168	THR	C-N-CA	5.54	130.00	122.07
1	B	278	SER	CA-C-O	5.54	126.41	120.20
1	A	201	ARG	CD-NE-CZ	5.53	132.14	124.40
1	C	153	ALA	O-C-N	5.53	128.45	122.15
1	C	93	ALA	CA-C-O	-5.52	115.12	121.47
1	B	153	ALA	CA-C-O	-5.50	115.01	120.90
1	A	177	HIS	CA-C-O	-5.49	113.78	120.54
1	C	233	HIS	CA-C-N	-5.49	113.49	122.54
1	C	233	HIS	C-N-CA	-5.49	113.49	122.54
1	B	210	ASP	CA-C-N	-5.48	113.27	121.87
1	B	210	ASP	C-N-CA	-5.48	113.27	121.87
1	A	303	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	A	5	ALA	CA-C-O	-5.46	115.38	121.23
1	C	258	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	138	SER	O-C-N	-5.42	115.88	122.22
1	C	293	GLN	CA-C-N	5.39	128.28	120.79
1	C	293	GLN	C-N-CA	5.39	128.28	120.79
1	B	290	ARG	CA-C-O	5.38	126.25	120.70
1	B	256	ASN	OD1-CG-ND2	5.38	127.98	122.60
1	B	152	ALA	CA-C-O	5.37	126.97	121.07
1	C	323	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	89	LEU	CA-C-O	5.35	125.03	119.14
1	A	114	ALA	CA-C-O	5.35	126.43	120.82
1	C	60	SER	O-C-N	-5.33	117.14	123.22
1	B	312	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	47	ALA	CA-C-O	5.29	126.03	120.42
1	A	106	GLY	O-C-N	-5.27	117.13	122.19
1	B	317	ILE	N-CA-CB	5.27	117.31	110.99
1	B	19	GLU	CB-CG-CD	5.26	121.55	112.60
1	A	133	GLU	CA-C-N	-5.23	111.86	122.31
1	A	133	GLU	C-N-CA	-5.23	111.86	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	PRO	CA-C-O	5.21	126.74	121.27
1	A	103	THR	CA-C-O	-5.19	115.53	121.40
1	C	268	ASP	O-C-N	5.18	129.19	122.40
1	C	312	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	89	LEU	CA-C-N	-5.18	117.09	122.89
1	B	89	LEU	C-N-CA	-5.18	117.09	122.89
1	B	253	LEU	CA-C-O	-5.18	115.55	121.40
1	C	201	ARG	CA-C-N	-5.17	113.43	121.18
1	C	201	ARG	C-N-CA	-5.17	113.43	121.18
1	C	272	THR	CA-C-N	-5.16	116.38	123.14
1	C	272	THR	C-N-CA	-5.16	116.38	123.14
1	A	308	GLN	CG-CD-NE2	-5.16	108.66	116.40
2	E	2	ILE	CA-C-O	-5.15	112.05	120.80
1	A	19	GLU	O-C-N	5.15	128.72	122.85
1	C	41	SER	CA-C-N	-5.14	112.98	120.29
1	C	41	SER	C-N-CA	-5.14	112.98	120.29
1	C	15	TYR	CA-C-O	5.11	125.61	119.43
1	C	222	SER	CA-C-O	-5.10	115.45	121.16
1	A	190	CYS	O-C-N	5.10	129.55	123.13
1	C	20	GLY	CA-C-O	5.08	124.66	119.02
1	C	219	GLY	N-CA-C	-5.06	104.84	111.37
1	B	44	GLN	CA-C-O	5.05	125.78	119.97
1	B	94	LYS	CA-C-N	5.05	129.49	122.77
1	B	94	LYS	C-N-CA	5.05	129.49	122.77
1	B	191	GLY	CA-C-N	-5.03	117.74	121.61
1	B	191	GLY	C-N-CA	-5.03	117.74	121.61
1	A	187	VAL	CA-C-O	5.03	126.45	120.72
1	C	273	VAL	CB-CA-C	5.03	118.07	110.63
1	C	262	GLY	N-CA-C	5.03	125.09	113.18
1	A	350	ARG	CA-C-O	5.02	125.74	120.42
1	A	262	GLY	O-C-N	5.01	129.03	122.71
1	A	24	GLN	CB-CG-CD	-5.01	104.08	112.60
1	C	127	ILE	CA-C-O	-5.01	115.05	120.36
1	B	351	LEU	CA-C-O	5.00	126.07	120.82
1	A	187	VAL	O-C-N	-5.00	118.04	123.14

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	38	0
1	B	2532	0	2419	47	0
1	C	2512	0	2396	61	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	13	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:HH11	1:A:223:ARG:HG2	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:171:GLU:HG3	5:C:2190:HOH:O	1.83	0.77
1:C:198:SER:O	1:C:201:ARG:HG3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:A:146:ARG:HH11	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:A:180:PHE:CG	1:A:181:PRO:HA	2.44	0.51
1:C:89:LEU:CD2	1:C:283:LEU:HD12	2.40	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:B:297:LYS:HG2	1:B:298:ALA:N	2.26	0.51
1:C:194:ARG:HD2	1:C:258:ASP:OD2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1943:HOH:O	1:B:315:HIS:HD2	1.95	0.50
1:A:142:ALA:O	1:A:146:ARG:HD3	2.12	0.49
1:A:223:ARG:HG2	1:A:223:ARG:NH1	2.16	0.49
1:A:303:ASN:HB2	1:A:304:PRO:HD3	1.94	0.49
1:B:44:GLN:O	1:B:48:SER:OG	2.29	0.49
1:B:108:LEU:O	1:B:112:THR:HG23	2.11	0.49
1:B:133:GLU:OE2	3:B:502:SO4:O4	2.30	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:A:173:ASP:CG	1:A:177:HIS:HE2	2.21	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:B:241:ASN:HA	1:B:242:PRO:HD3	1.77	0.47
1:C:291:ILE:HG21	1:C:355:LEU:HD12	1.97	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:HE2	1:A:121:LYS:HB2	1.58	0.47
1:A:350:ARG:NE	5:A:1519:HOH:O	2.48	0.46
1:C:9:LEU:CD1	1:C:49:LEU:HD22	2.35	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:210:ASP:OD2	1:C:258:ASP:OD1	2.33	0.46
1:C:243:GLY:HA3	5:C:2314:HOH:O	2.14	0.46
1:C:294:LYS:HD2	1:C:294:LYS:HA	1.74	0.46
1:C:303:ASN:HB2	1:C:304:PRO:HD3	1.98	0.46
1:A:146:ARG:HG3	1:A:146:ARG:NH1	2.28	0.46
1:A:260:ALA:HB2	1:B:312:ASP:HB3	1.98	0.46
1:B:136:TRP:HB2	1:B:141:ILE:HD11	1.98	0.46
1:C:4:THR:N	1:C:260:ALA:O	2.49	0.46
1:B:194:ARG:NH1	5:B:2408:HOH:O	2.49	0.45
1:C:13:GLN:NE2	5:C:2113:HOH:O	2.49	0.45
1:C:323:ASP:N	5:C:2013:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:315:HIS:HE1	5:B:2138:HOH:O	2.00	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: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:B:45:TYR:CE2	1:B:84:GLU:HB3	2.52	0.44
1:C:273:VAL:C	1:C:274:ILE:HD13	2.42	0.44
1:C:281:ALA:HB3	1:C:282:PRO:HD3	2.00	0.44
1:C:322:ASN:N	5:C:2013:HOH:O	2.49	0.44
1:B:22:ASP:HB2	1:B:91:PRO:HG2	1.99	0.44
1:A:194:ARG:NH1	5:A:2101:HOH:O	2.49	0.44
1:B:239:SER:HB3	1:B:244:ALA:HB3	2.00	0.44
1:A:146:ARG:NH1	5:A:1925:HOH:O	2.50	0.44
1:B:213:ASP:HB2	5:B:2065:HOH:O	2.17	0.44
1:C:194:ARG:NH1	5:C:1963:HOH:O	2.50	0.44
1:C:291:ILE:HD13	1:C:355:LEU:HD12	1.99	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:16:GLN:NE2	5:A:1887:HOH:O	2.50	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:B:297:LYS:HB3	1:B:297:LYS:HE3	1.14	0.43
1:C:290:ARG:O	1:C:293:GLN:HB3	2.18	0.43
1:C:224:ILE:N	1:C:224:ILE:HD13	2.34	0.43
1:C:228:PRO:HA	5:C:2253:HOH:O	2.18	0.43
1:C:292:ASN:CG	1:C:298:ALA:HA	2.44	0.43
1:A:62:ASP:OD2	1:A:109:ASP:OD2	2.37	0.42
1:A:309:LEU:HD22	1:A:354:ALA:HB1	2.01	0.42
1:B:5:ALA:HB1	1:B:264:GLU:HG3	2.01	0.42
1:C:297:LYS:O	1:C:297:LYS:HG2	2.18	0.42
1:A:224:ILE:HD13	1:A:224:ILE:N	2.34	0.42
1:B:229:ALA:HA	1:B:232:GLU:HG2	2.02	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:279:ALA:C	1:A:282:PRO:HD2	2.45	0.42
1:A:30:ILE:HG21	1:A:30:ILE:HD13	1.80	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLU:OE1	1:C:19:GLU:HA	2.16	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:62:ASP:OD2	1:B:109:ASP:OD2	2.40	0.40
1:B:239:SER:HB3	1:B:244:ALA:HB1	2.03	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

5.3.1 Protein backbone

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
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%)	235 (93%)	18 (7%)	13	4
1	B	253/260 (97%)	239 (94%)	14 (6%)	19	8
1	C	251/260 (96%)	218 (87%)	33 (13%)	4	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%)	10	3

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

Mol	Chain	Res	Type
1	A	49	LEU
1	A	89	LEU
1	A	134	ASP
1	A	141	ILE
1	A	146	ARG
1	A	168	THR
1	A	172	GLN
1	A	194	ARG
1	A	201	ARG
1	A	213	ASP
1	A	223	ARG
1	A	224	ILE
1	A	242	PRO
1	A	246	SER
1	A	251	PRO
1	A	297	LYS
1	A	302	LEU
1	A	332	GLN
1	B	4	THR
1	B	51	VAL
1	B	89	LEU
1	B	144	MET

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Mol	Chain	Res	Type
1	B	168	THR
1	B	172	GLN
1	B	188	LEU
1	B	223	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	89	LEU
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	194	ARG
1	C	201	ARG
1	C	223	ARG
1	C	224	ILE
1	C	232	GLU
1	C	235	ASN
1	C	245	SER
1	C	264	GLU
1	C	270	GLU
1	C	274	ILE
1	C	291	ILE
1	C	297	LYS
1	C	308	GLN
1	C	319	GLU
1	C	324	ILE
1	C	326	ASN
1	C	327	ARG

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Mol	Chain	Res	Type
1	C	353	GLN

Sometimes 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	55	GLN
1	A	145	ASN
1	A	172	GLN
1	A	303	ASN
1	A	315	HIS
1	A	332	GLN
1	B	44	GLN
1	B	55	GLN
1	B	116	HIS
1	B	145	ASN
1	B	204	GLN
1	B	256	ASN
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	116	HIS
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	2,1	11,11,11	0.58	0	11,13,13	0.70	0
2	PHL	F	4	2,1	11,11,11	0.50	0	11,13,13	0.70	0
2	PHL	E	4	2,1	11,11,11	0.46	0	11,13,13	0.84	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	2,1	-	3/6/6/6	0/1/1/1
2	PHL	F	4	2,1	-	2/6/6/6	0/1/1/1
2	PHL	E	4	2,1	-	3/6/6/6	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	PHL	CA-CB-CG-CD2
2	E	4	PHL	CA-CB-CG-CD1
2	D	4	PHL	O-C-CA-N
2	E	4	PHL	O-C-CA-N
2	D	4	PHL	CA-CB-CG-CD2
2	D	4	PHL	CA-CB-CG-CD1
2	F	4	PHL	CA-CB-CG-CD2
2	F	4	PHL	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	502	-	4,4,4	0.39	0	6,6,6	0.29	0
3	SO4	C	503	-	4,4,4	0.42	0	6,6,6	0.28	0
3	SO4	A	501	-	4,4,4	0.42	0	6,6,6	0.31	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.55	0 100 100	11, 18, 35, 60	0
1	B	356/364 (97%)	-0.60	2 (0%) 85 86	11, 19, 36, 63	0
1	C	353/364 (96%)	-0.13	2 (0%) 85 86	13, 28, 54, 82	0
2	D	2/4 (50%)	-0.48	0 100 100	15, 15, 15, 21	0
2	E	2/4 (50%)	-0.92	0 100 100	18, 18, 18, 19	0
2	F	2/4 (50%)	-0.58	0 100 100	20, 20, 20, 24	0
All	All	1072/1104 (97%)	-0.43	4 (0%) 88 89	11, 21, 43, 82	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	THR	3.0
1	B	2	ALA	3.0
1	B	3	PRO	2.9
1	C	201	ARG	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PHL	D	4	11/11	0.95	0.06	7,14,20,23	0
2	PHL	E	4	11/11	0.96	0.05	9,16,18,20	0
2	PHL	F	4	11/11	0.96	0.05	18,22,27,28	0

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
3	SO4	C	503	5/5	0.78	0.17	41,68,70,103	0
3	SO4	A	501	5/5	0.90	0.10	30,46,58,68	0
3	SO4	B	502	5/5	0.97	0.07	32,33,37,38	0
4	CA	C	603	1/1	0.97	0.04	41,41,41,41	0
4	CA	A	601	1/1	0.98	0.03	18,18,18,18	0
4	CA	B	602	1/1	0.99	0.03	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.