



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:32 PM GMT

PDB ID : 4FBL
Title : LipS and LipT, two metagenome-derived lipolytic enzymes increase the diversity of known lipase and esterase families
Authors : Chow, J.; Krauss, U.; Dall Antonia, Y.; Fersini, F.; Schmeisser, C.; Schmidt, M.; Menyes, I.; Bornscheuer, U.; Lauinger, B.; Bongen, P.; Pietruszka, J.; Eckstein, M.; Thum, O.; Liese, A.; Mueller-Dieckmann, J.; Jaeger, K.-E.; Kovacic, F.; Streit, W.R.; Structural Proteomics in Europe (SPINE)
Deposited on : 2012-05-23
Resolution : 1.99 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

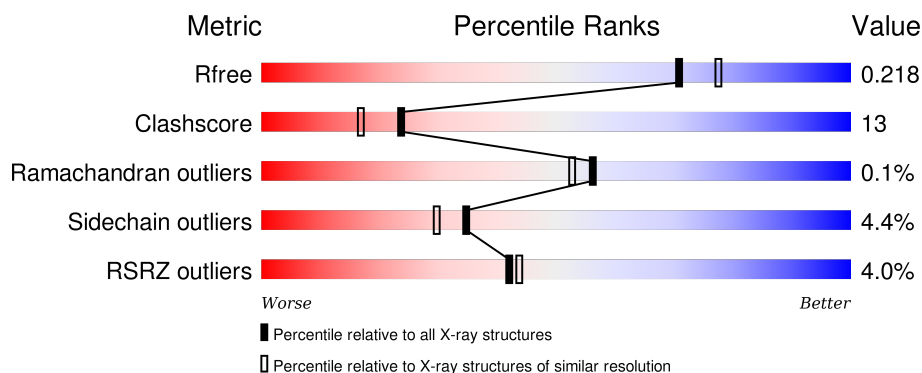
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	281	<div> <div>70%</div> <div>16%</div> <div>13%</div> </div>
1	B	281	<div> <div>72%</div> <div>13%</div> <div>12%</div> </div>
1	C	281	<div> <div>69%</div> <div>16%</div> <div>12%</div> </div>
1	D	281	<div> <div>69%</div> <div>16%</div> <div>12%</div> </div>

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
2	SPD	A	301	-	-	X	X
2	SPD	B	301	-	-	X	-
2	SPD	C	301	-	-	X	-
3	CL	A	302	-	-	X	-
3	CL	B	302	-	-	X	-
3	CL	C	302	-	-	X	-
3	CL	D	301	-	-	X	-

2 Entry composition [i](#)

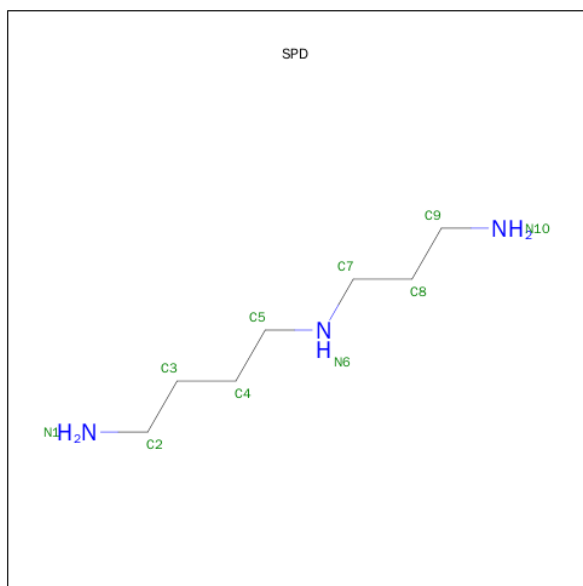
There are 4 unique types of molecules in this entry. The entry contains 8087 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LipS lipolytic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1850	1182	316	342	10			
1	B	246	Total	C	N	O	S	0	1	0
			1861	1190	315	346	10			
1	C	246	Total	C	N	O	S	0	1	0
			1867	1193	318	346	10			
1	D	246	Total	C	N	O	S	0	1	0
			1867	1193	318	346	10			

- Molecule 2 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			10	7	3		
2	B	1	Total	C	N	0	0
			10	7	3		

Continued on next page...

Continued from previous page...

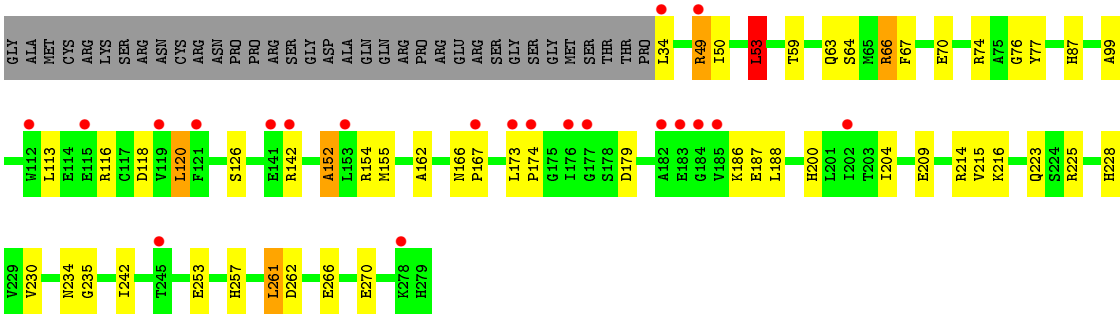
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	N	0	0
			10	7	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	153	Total	O	0	0
			153	153		
4	B	164	Total	O	0	0
			164	164		
4	C	169	Total	O	0	0
			169	169		
4	D	122	Total	O	0	0
			122	122		



4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	105.27Å 105.27Å 120.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.30 – 1.99 40.33 – 1.99	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.30-1.99) 100.0 (40.33-1.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.176 , 0.217 0.178 , 0.218	Depositor DCC
R_{free} test set	4524 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.1	EDS
Estimated twinning fraction	0.076 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 90469 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8087	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, 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	A	1.38	4/1895 (0.2%)	1.09	4/2583 (0.2%)
1	B	1.33	5/1906 (0.3%)	1.06	6/2600 (0.2%)
1	C	1.34	4/1912 (0.2%)	1.15	13/2607 (0.5%)
1	D	1.25	1/1912 (0.1%)	1.03	5/2607 (0.2%)
All	All	1.33	14/7625 (0.2%)	1.08	28/10397 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	CYS	CB-SG	-8.09	1.68	1.82
1	B	270	GLU	CG-CD	5.90	1.60	1.51
1	B	77	TYR	CD2-CE2	5.84	1.48	1.39
1	D	152	ALA	CA-CB	5.66	1.64	1.52
1	C	72	PHE	CE2-CZ	5.63	1.48	1.37
1	A	226	GLU	CG-CD	5.62	1.60	1.51
1	A	165	PHE	CE2-CZ	5.61	1.48	1.37
1	B	117	CYS	CB-SG	-5.59	1.72	1.81
1	C	209	GLU	CG-CD	5.51	1.60	1.51
1	B	270	GLU	CD-OE2	5.49	1.31	1.25
1	A	158	PRO	N-CA	5.45	1.56	1.47
1	A	190	TYR	CD2-CE2	5.26	1.47	1.39
1	B	277	ARG	CG-CD	5.10	1.64	1.51
1	C	58	PHE	CE1-CZ	5.10	1.47	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	ARG	NE-CZ-NH2	-11.39	114.60	120.30
1	C	214	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	A	265	LYS	CD-CE-NZ	-9.56	89.72	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	B	271	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	C	173	LEU	CA-CB-CG	7.31	132.11	115.30
1	C	277	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	C	277	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	C	65	MET	CG-SD-CE	6.71	110.94	100.20
1	C	74	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	C	83	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	154	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	D	214	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	111	ARG	CG-CD-NE	5.88	124.14	111.80
1	D	120	LEU	CA-CB-CG	5.86	128.78	115.30
1	C	120	LEU	CB-CG-CD1	5.76	120.79	111.00
1	D	214	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	C	250	LEU	CB-CG-CD2	-5.57	101.54	111.00
1	B	265	LYS	CD-CE-NZ	-5.50	99.06	111.70
1	C	179	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	261	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	277	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	68	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	C	74	ARG	CG-CD-NE	-5.28	100.71	111.80
1	D	262	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	53	LEU	CA-CB-CG	5.10	127.03	115.30
1	B	271	ARG	CG-CD-NE	-5.09	101.11	111.80
1	C	277	ARG	CB-CA-C	-5.07	100.26	110.40

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	1850	0	1853	45	0
1	B	1861	0	1859	48	0
1	C	1867	0	1870	46	0
1	D	1867	0	1870	47	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	19	21	0
2	B	10	0	19	14	0
2	C	10	0	19	18	0
3	A	1	0	0	4	0
3	B	1	0	0	4	0
3	C	1	0	0	3	0
3	D	1	0	0	2	0
4	A	153	0	0	4	0
4	B	164	0	0	4	0
4	C	169	0	0	6	0
4	D	122	0	0	5	0
All	All	8087	0	7509	198	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 13.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ILE:HG12	2:A:301:SPD:H42	1.26	1.14
1:B:114:GLU:HG2	1:B:142:ARG:HH21	1.05	1.08
1:C:63:GLN:HG2	1:C:188:LEU:HB3	1.16	1.07
1:B:155:MET:CE	1:B:155:MET:HA	1.89	1.02
1:D:63:GLN:HG2	1:D:188:LEU:HB3	1.37	1.01
1:A:257:HIS:NE2	2:A:301:SPD:N10	2.08	1.01
1:B:114:GLU:HG2	1:B:142:ARG:NH2	1.76	1.00
1:B:167:PRO:HD3	4:B:503:HOH:O	1.60	0.99
1:A:177:GLY:N	2:A:301:SPD:C2	2.27	0.97
1:B:155:MET:HA	1:B:155:MET:HE3	1.47	0.96
1:B:111:ARG:HH11	1:B:111:ARG:HG3	1.30	0.94
3:A:302:CL:CL	4:A:495:HOH:O	2.23	0.92
1:C:63:GLN:HG2	1:C:188:LEU:CB	2.00	0.92
1:A:177:GLY:N	2:A:301:SPD:H21	1.85	0.92
1:B:257:HIS:NE2	2:B:301:SPD:N10	2.19	0.89
1:C:257:HIS:HD2	2:C:301:SPD:H32	1.37	0.88
1:A:177:GLY:N	2:A:301:SPD:H22	1.88	0.88
1:D:154:ARG:H	1:D:234:ASN:HD21	1.19	0.86
1:C:257:HIS:NE2	2:C:301:SPD:N10	2.24	0.86
1:B:59:THR:H	1:B:87:HIS:HE1	1.23	0.86
3:C:302:CL:CL	4:C:568:HOH:O	2.32	0.84
1:A:154:ARG:H	1:A:234:ASN:HD21	1.22	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:SER:OG	1:D:257:HIS:NE2	2.11	0.83
1:A:177:GLY:CA	2:A:301:SPD:H22	2.08	0.83
3:B:302:CL:CL	4:B:488:HOH:O	2.33	0.83
1:A:126:SER:OG	1:A:257:HIS:CE1	2.34	0.81
1:C:126:SER:OG	1:C:257:HIS:NE2	2.13	0.81
1:B:187:GLU:OE1	2:B:301:SPD:H42	1.81	0.80
3:D:301:CL:CL	4:D:464:HOH:O	2.35	0.80
1:B:126:SER:OG	1:B:257:HIS:NE2	2.15	0.80
1:B:126:SER:OG	1:B:257:HIS:CE1	2.36	0.79
1:C:179:ASP:H	2:C:301:SPD:HN12	1.29	0.79
1:D:63:GLN:NE2	1:D:188:LEU:H	1.83	0.77
1:B:59:THR:H	1:B:87:HIS:CE1	2.03	0.77
1:B:126:SER:OG	2:B:301:SPD:N10	2.18	0.76
1:B:179:ASP:H	2:B:301:SPD:HN12	1.30	0.76
1:C:126:SER:HB3	3:C:302:CL:CL	2.22	0.76
2:A:301:SPD:H91	3:A:302:CL:CL	2.22	0.75
1:B:154:ARG:H	1:B:234:ASN:HD21	1.32	0.75
1:C:200:HIS:HE1	4:C:522:HOH:O	1.70	0.74
1:C:110:MET:HE2	1:C:142:ARG:HH11	1.51	0.74
1:C:176:ILE:O	2:C:301:SPD:H22	1.87	0.74
1:B:155:MET:HA	1:B:155:MET:HE2	1.70	0.73
1:D:63:GLN:HG2	1:D:188:LEU:CB	2.15	0.73
1:D:126:SER:OG	1:D:257:HIS:CE1	2.43	0.72
1:D:126:SER:HB3	3:D:301:CL:CL	2.27	0.72
1:A:126:SER:OG	1:A:257:HIS:NE2	2.23	0.72
1:C:154:ARG:NH1	1:C:156:GLU:OE2	2.23	0.72
1:C:187:GLU:OE1	2:C:301:SPD:H42	1.91	0.71
1:B:35:GLN:HG3	1:C:184:GLY:O	1.91	0.71
2:C:301:SPD:H91	3:C:302:CL:CL	2.28	0.71
1:C:179:ASP:OD1	1:C:228:HIS:HD2	1.74	0.70
1:A:176:ILE:HG12	2:A:301:SPD:C4	2.15	0.70
1:A:126:SER:HB3	3:A:302:CL:CL	2.29	0.69
1:D:154:ARG:NE	1:D:209:GLU:OE1	2.25	0.69
1:C:66:ARG:O	1:C:70:GLU:HG2	1.92	0.69
1:B:126:SER:HG	2:B:301:SPD:H102	1.41	0.69
1:D:155:MET:HE1	1:D:230:VAL:HG22	1.73	0.69
1:B:114:GLU:CG	1:B:142:ARG:HH21	1.96	0.68
1:B:176:ILE:O	2:B:301:SPD:H22	1.93	0.68
2:B:301:SPD:H91	3:B:302:CL:CL	2.31	0.68
1:D:59:THR:H	1:D:87:HIS:CE1	2.12	0.67
1:B:126:SER:HB3	3:B:302:CL:CL	2.32	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:SER:OG	2:C:301:SPD:N10	2.28	0.67
1:D:64:SER:HB3	4:D:467:HOH:O	1.94	0.66
1:C:179:ASP:N	2:C:301:SPD:HN12	1.93	0.66
1:B:63:GLN:CG	1:B:188:LEU:HB3	2.25	0.66
1:A:176:ILE:C	2:A:301:SPD:H21	2.15	0.66
1:D:215:VAL:HG11	1:D:242:ILE:HD11	1.77	0.65
1:A:56:HIS:HE1	1:A:84:LEU:H	1.45	0.65
1:A:177:GLY:H	2:A:301:SPD:C2	2.08	0.65
2:C:301:SPD:H41	2:C:301:SPD:C8	2.24	0.65
1:C:154:ARG:H	1:C:234:ASN:HD21	1.44	0.64
1:C:63:GLN:NE2	1:C:188:LEU:H	1.95	0.64
1:D:63:GLN:CG	1:D:188:LEU:HB3	2.20	0.63
1:D:59:THR:H	1:D:87:HIS:HE1	1.47	0.63
1:D:270:GLU:HG2	4:D:496:HOH:O	1.99	0.63
1:D:66:ARG:O	1:D:70:GLU:HG2	1.99	0.63
1:B:63:GLN:HG3	1:B:188:LEU:HB3	1.82	0.62
1:C:63:GLN:CG	1:C:188:LEU:HB3	2.10	0.61
1:C:126:SER:OG	1:C:257:HIS:CE1	2.53	0.60
1:A:126:SER:OG	2:A:301:SPD:N10	2.34	0.60
1:B:107:VAL:O	1:B:111:ARG:HG2	2.02	0.60
1:A:177:GLY:HA3	2:A:301:SPD:H22	1.82	0.60
1:A:49:ARG:HG3	4:A:410:HOH:O	2.02	0.59
1:B:111:ARG:HH11	1:B:111:ARG:CG	2.10	0.58
1:A:59:THR:OG1	2:A:301:SPD:H32	2.04	0.58
1:D:66:ARG:HD2	4:D:521:HOH:O	2.03	0.58
1:D:49:ARG:HG3	1:D:118:ASP:OD2	2.04	0.57
1:D:225:ARG:HH21	1:D:253:GLU:CD	2.08	0.57
1:A:177:GLY:CA	2:A:301:SPD:C2	2.79	0.57
1:B:172:GLU:O	1:B:173:LEU:HD23	2.04	0.57
1:C:179:ASP:HB3	2:C:301:SPD:N1	2.20	0.56
1:D:99:ALA:H	1:D:200:HIS:CD2	2.23	0.56
1:D:223:GLN:NE2	4:D:431:HOH:O	2.38	0.56
1:D:99:ALA:HB1	1:D:204:ILE:HD11	1.87	0.56
1:D:50:ILE:HB	1:D:77:TYR:HD1	1.70	0.56
1:D:173:LEU:HB3	1:D:174:PRO:HD2	1.88	0.55
1:A:177:GLY:H	2:A:301:SPD:H22	1.65	0.55
1:B:169:ALA:HB1	1:B:170:PRO:HD2	1.88	0.55
1:B:61:SER:HB2	1:B:62:PRO:HD2	1.88	0.55
1:C:59:THR:H	1:C:87:HIS:HE1	1.53	0.55
1:C:126:SER:HG	2:C:301:SPD:H102	1.54	0.55
1:A:233:HIS:HD2	1:A:236:GLU:OE1	1.90	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:MET:CE	1:C:142:ARG:HH11	2.18	0.54
1:A:41:GLU:HB2	1:A:42:PRO:HD2	1.89	0.54
1:B:59:THR:N	1:B:87:HIS:HE1	1.98	0.54
1:A:56:HIS:CE1	1:A:84:LEU:H	2.25	0.54
1:B:257:HIS:HD2	2:B:301:SPD:H32	1.73	0.53
1:D:155:MET:CE	1:D:230:VAL:HG22	2.38	0.53
1:D:179:ASP:OD1	1:D:228:HIS:HD2	1.91	0.52
1:C:242:ILE:HD12	1:C:244:SER:HB2	1.91	0.52
1:D:152:ALA:HB1	1:D:155:MET:HE1	1.91	0.52
1:A:176:ILE:CA	2:A:301:SPD:H21	2.39	0.52
2:A:301:SPD:H71	4:A:423:HOH:O	2.10	0.52
1:D:223:GLN:HG3	1:D:235:GLY:HA3	1.90	0.52
2:C:301:SPD:C5	2:C:301:SPD:H92	2.40	0.52
1:B:63:GLN:HG2	1:B:188:LEU:HB3	1.90	0.52
1:D:154:ARG:H	1:D:234:ASN:ND2	1.99	0.51
1:C:257:HIS:CD2	2:C:301:SPD:N10	2.78	0.51
1:B:154:ARG:N	1:B:234:ASN:HD21	2.04	0.51
1:C:187:GLU:OE2	2:C:301:SPD:H71	2.09	0.51
1:B:59:THR:N	1:B:87:HIS:CE1	2.77	0.51
1:A:126:SER:HG	2:A:301:SPD:H101	1.55	0.50
1:C:59:THR:H	1:C:87:HIS:CE1	2.29	0.50
1:A:56:HIS:HD2	1:A:57:GLY:O	1.95	0.49
1:C:43:LEU:HD12	1:C:43:LEU:C	2.33	0.49
1:A:99:ALA:H	1:A:200:HIS:CD2	2.30	0.49
1:A:147:MET:HA	1:A:220:LEU:O	2.13	0.49
1:D:63:GLN:HE22	1:D:187:GLU:HA	1.78	0.49
1:A:41:GLU:H	1:A:41:GLU:CD	2.16	0.49
2:C:301:SPD:H72	4:C:441:HOH:O	2.10	0.49
1:D:152:ALA:CB	1:D:155:MET:HE1	2.42	0.49
1:D:152:ALA:HB1	1:D:155:MET:CE	2.43	0.48
1:B:155:MET:HE2	1:B:155:MET:CA	2.36	0.48
1:A:233:HIS:CD2	1:A:236:GLU:OE1	2.66	0.48
1:B:186:LYS:HE3	1:B:187:GLU:O	2.13	0.48
1:A:166:ASN:HB3	1:A:169:ALA:HB2	1.95	0.48
1:A:35:GLN:OE1	1:A:35:GLN:HA	2.14	0.47
1:A:257:HIS:CD2	2:A:301:SPD:N10	2.81	0.47
1:B:184:GLY:O	1:C:35:GLN:HG3	2.14	0.47
1:D:215:VAL:HB	1:D:242:ILE:HG13	1.96	0.47
1:B:61:SER:HB2	1:B:62:PRO:CD	2.44	0.47
1:C:179:ASP:CB	2:C:301:SPD:HN12	2.28	0.47
1:D:49:ARG:CG	1:D:118:ASP:OD2	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ASP:OD1	4:C:464:HOH:O	2.21	0.47
1:A:126:SER:HG	1:A:257:HIS:CE1	2.28	0.46
1:D:225:ARG:NH2	1:D:253:GLU:OE2	2.43	0.46
1:C:110:MET:CE	1:C:142:ARG:HD2	2.46	0.46
1:C:99:ALA:H	1:C:200:HIS:CD2	2.34	0.46
1:D:162:ALA:O	1:D:166:ASN:HB2	2.16	0.45
1:C:179:ASP:OD1	1:C:228:HIS:CD2	2.63	0.45
1:C:147:MET:HA	1:C:220:LEU:O	2.15	0.45
1:C:231:PRO:HA	1:C:232:PRO:HD3	1.77	0.45
1:B:142:ARG:HD2	1:B:142:ARG:O	2.16	0.45
1:D:204:ILE:HG23	1:D:204:ILE:HD12	1.72	0.45
2:A:301:SPD:H41	2:A:301:SPD:H92	1.98	0.45
1:B:155:MET:HE1	1:B:230:VAL:HA	1.97	0.45
1:B:178:SER:H	2:B:301:SPD:H21	1.82	0.45
1:B:126:SER:CB	2:B:301:SPD:N10	2.81	0.44
1:C:110:MET:CE	1:C:142:ARG:CD	2.96	0.44
1:B:43:LEU:HD11	1:B:70:GLU:HG3	2.00	0.44
1:C:180:ILE:HG21	1:C:185:VAL:HB	1.98	0.44
1:D:166:ASN:HA	1:D:167:PRO:HD2	1.89	0.44
2:B:301:SPD:H72	4:B:419:HOH:O	2.17	0.44
1:D:74:ARG:C	1:D:76:GLY:H	2.19	0.44
1:D:154:ARG:N	1:D:234:ASN:HD21	1.99	0.43
1:B:229:VAL:HG21	2:B:301:SPD:HN11	1.83	0.43
1:D:64:SER:O	1:D:261:LEU:HD13	2.18	0.43
1:A:67:PHE:CE2	1:A:265:LYS:HG3	2.54	0.43
1:A:114:GLU:OE2	1:A:142:ARG:HD3	2.18	0.43
1:C:257:HIS:CD2	2:C:301:SPD:H32	2.30	0.43
1:C:200:HIS:CE1	4:C:522:HOH:O	2.56	0.43
1:C:63:GLN:HE21	1:C:188:LEU:H	1.64	0.43
2:B:301:SPD:H41	2:B:301:SPD:H71	1.31	0.43
1:D:53:LEU:HB2	1:D:113:LEU:CD1	2.49	0.42
1:A:161:ALA:HB2	1:C:210:MET:HB3	2.01	0.42
1:D:67:PHE:CZ	1:D:266:GLU:HG3	2.55	0.42
1:D:215:VAL:HB	1:D:242:ILE:CG1	2.49	0.42
1:B:126:SER:HG	1:B:257:HIS:CE1	2.23	0.42
1:C:178:SER:N	2:C:301:SPD:H21	2.34	0.42
1:D:63:GLN:NE2	1:D:187:GLU:HA	2.35	0.42
1:D:59:THR:N	1:D:87:HIS:CE1	2.86	0.42
1:B:138:GLN:NE2	4:B:415:HOH:O	2.53	0.42
1:A:214:ARG:HD2	4:C:464:HOH:O	2.20	0.41
1:A:126:SER:HA	1:A:150:ASN:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:PHE:HB3	3:A:302:CL:CL	2.57	0.41
1:B:58:PHE:HB3	3:B:302:CL:CL	2.57	0.41
1:C:66:ARG:HG3	1:C:66:ARG:NH1	2.36	0.41
1:A:149:ILE:HA	1:A:222:ILE:O	2.20	0.41
2:A:301:SPD:C5	2:A:301:SPD:H92	2.51	0.41
1:A:231:PRO:HA	1:A:232:PRO:HD3	1.94	0.41
1:A:218:PRO:HB3	1:A:246:GLU:HG2	2.02	0.41
1:A:176:ILE:HG21	1:A:176:ILE:HD13	1.71	0.41
1:B:155:MET:CE	1:B:155:MET:CA	2.71	0.40
1:B:177:GLY:CA	2:B:301:SPD:H22	2.51	0.40
1:D:186:LYS:HB3	1:D:186:LYS:HE3	1.99	0.40
1:A:265:LYS:HE3	4:A:409:HOH:O	2.20	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	243/281 (86%)	232 (96%)	11 (4%)	0	100	100
1	B	245/281 (87%)	235 (96%)	9 (4%)	1 (0%)	39	33
1	C	245/281 (87%)	236 (96%)	9 (4%)	0	100	100
1	D	245/281 (87%)	234 (96%)	11 (4%)	0	100	100
All	All	978/1124 (87%)	937 (96%)	40 (4%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	PRO

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	193/223 (86%)	184 (95%)	9 (5%)	32	27
1	B	194/223 (87%)	188 (97%)	6 (3%)	47	46
1	C	195/223 (87%)	185 (95%)	10 (5%)	29	23
1	D	195/223 (87%)	186 (95%)	9 (5%)	33	28
All	All	777/892 (87%)	743 (96%)	34 (4%)	35	30

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	49	ARG
1	A	53	LEU
1	A	93	GLU
1	A	176	ILE
1	A	183	GLU
1	A	186	LYS
1	A	216	LYS
1	A	265	LYS
1	B	63	GLN
1	B	111	ARG
1	B	142	ARG
1	B	155	MET
1	B	186	LYS
1	B	218	PRO
1	C	43	LEU
1	C	63	GLN
1	C	173	LEU
1	C	174	PRO
1	C	178	SER
1	C	183	GLU
1	C	186	LYS
1	C	237	LEU
1	C	261	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	278	LYS
1	D	34	LEU
1	D	49	ARG
1	D	53	LEU
1	D	66	ARG
1	D	116	ARG
1	D	120	LEU
1	D	142	ARG
1	D	216	LYS
1	D	261	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	200	HIS
1	A	233	HIS
1	A	234	ASN
1	A	263	ASN
1	B	87	HIS
1	B	138	GLN
1	B	200	HIS
1	B	234	ASN
1	C	63	GLN
1	C	87	HIS
1	C	200	HIS
1	C	228	HIS
1	C	234	ASN
1	D	63	GLN
1	D	87	HIS
1	D	200	HIS
1	D	223	GLN
1	D	228	HIS
1	D	234	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 4 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	$\# Z > 2$
2	SPD	A	301	-	9,9,9	0.81	0	8,8,8	1.54	1 (12%)
2	SPD	B	301	-	9,9,9	0.51	0	8,8,8	1.97	3 (37%)
2	SPD	C	301	-	9,9,9	0.67	0	8,8,8	1.24	1 (12%)

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	SPD	A	301	-	-	0/7/7/7	0/0/0/0
2	SPD	B	301	-	-	0/7/7/7	0/0/0/0
2	SPD	C	301	-	-	0/7/7/7	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	SPD	C4-C5-N6	-3.46	103.32	111.96
2	B	301	SPD	C8-C7-N6	-2.86	104.82	111.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	SPD	C4-C5-N6	-2.35	106.08	111.96
2	B	301	SPD	C7-N6-C5	2.54	122.34	113.35
2	A	301	SPD	C7-N6-C5	3.27	124.93	113.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	SPD	21	0
2	B	301	SPD	14	0
2	C	301	SPD	18	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	245/281 (87%)	-0.01	4 (1%) 74 75	12, 23, 37, 50	0
1	B	246/281 (87%)	0.03	7 (2%) 56 57	14, 24, 46, 58	0
1	C	246/281 (87%)	0.10	7 (2%) 56 57	15, 24, 39, 52	0
1	D	246/281 (87%)	0.43	21 (8%) 13 14	19, 34, 50, 59	0
All	All	983/1124 (87%)	0.14	39 (3%) 42 44	12, 26, 46, 59	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	LEU	5.2
1	C	34	LEU	4.7
1	B	168	ASP	4.2
1	D	183	GLU	3.9
1	D	185	VAL	3.4
1	C	176	ILE	3.3
1	D	173	LEU	3.3
1	C	175	GLY	3.2
1	B	167	PRO	3.0
1	A	176	ILE	3.0
1	D	34	LEU	3.0
1	D	176	ILE	2.8
1	B	176	ILE	2.7
1	D	115	GLU	2.7
1	B	174	PRO	2.7
1	A	183	GLU	2.7
1	D	184	GLY	2.5
1	D	49	ARG	2.4
1	D	142	ARG	2.4
1	B	175	GLY	2.4
1	B	177	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	121	PHE	2.4
1	D	245	THR	2.4
1	D	278	LYS	2.4
1	A	168	ASP	2.3
1	D	177	GLY	2.3
1	D	202	ILE	2.3
1	D	153	LEU	2.2
1	D	112	TRP	2.2
1	A	35	GLN	2.2
1	C	183	GLU	2.2
1	D	119	VAL	2.1
1	D	174	PRO	2.1
1	D	141	GLU	2.1
1	C	177	GLY	2.1
1	C	184	GLY	2.1
1	C	153	LEU	2.0
1	D	167	PRO	2.0
1	D	182	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	SPD	A	301	10/10	0.80	0.24	2.97	25,43,50,52	0
2	SPD	C	301	10/10	0.83	0.20	1.59	30,41,48,49	0
2	SPD	B	301	10/10	0.87	0.18	1.19	32,37,44,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CL	A	302	1/1	0.99	0.07	-1.57	29,29,29,29	0
3	CL	B	302	1/1	0.99	0.07	-1.84	35,35,35,35	0
3	CL	C	302	1/1	0.99	0.07	-2.06	34,34,34,34	0
3	CL	D	301	1/1	0.99	0.07	-3.67	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.