



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:53 PM UTC

PDB ID : 4FBL / pdb_00004fbl
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

<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)

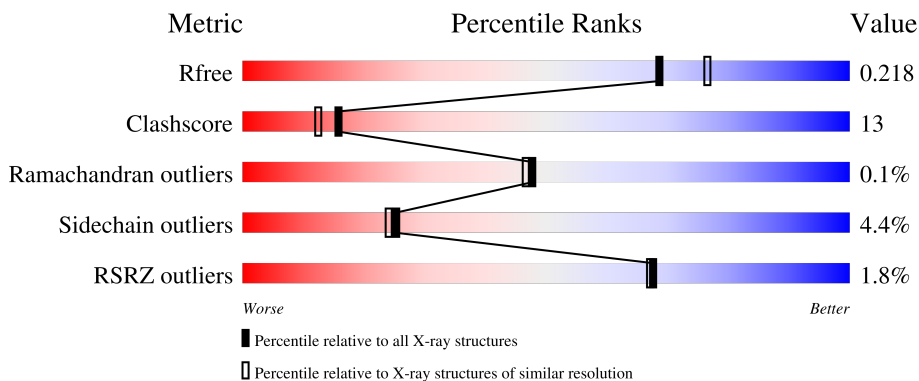
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	281	 2% 68% 18% • 13%
1	B	281	 2% 69% 16% • 12%
1	C	281	 2% 66% 19% • 12%
1	D	281	 2% 64% 19% • 12%

Validation Pipeline (wwPDB-VP) : 2.49

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	-
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](#)

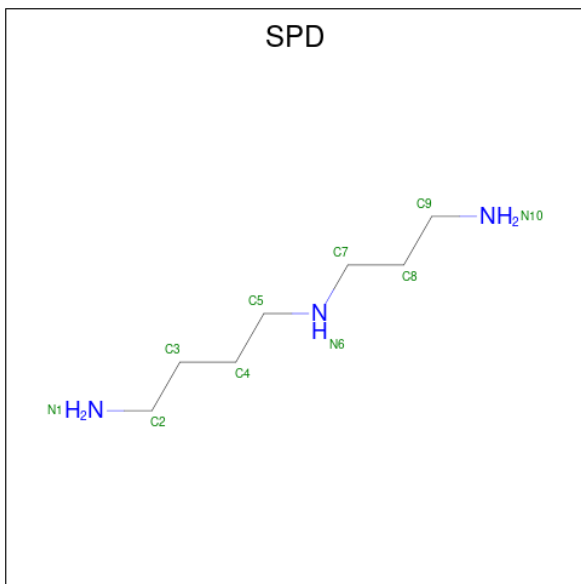
There are 4 unique types of molecules in this entry. The entry contains 8087 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	245	Total 1850	C 1182	N 316	O 342	S 10	0	0	0
1	B	246	Total 1861	C 1190	N 315	O 346	S 10	0	1	0
1	C	246	Total 1867	C 1193	N 318	O 346	S 10	0	1	0
1	D	246	Total 1867	C 1193	N 318	O 346	S 10	0	1	0

- Molecule 2 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



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

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is water.

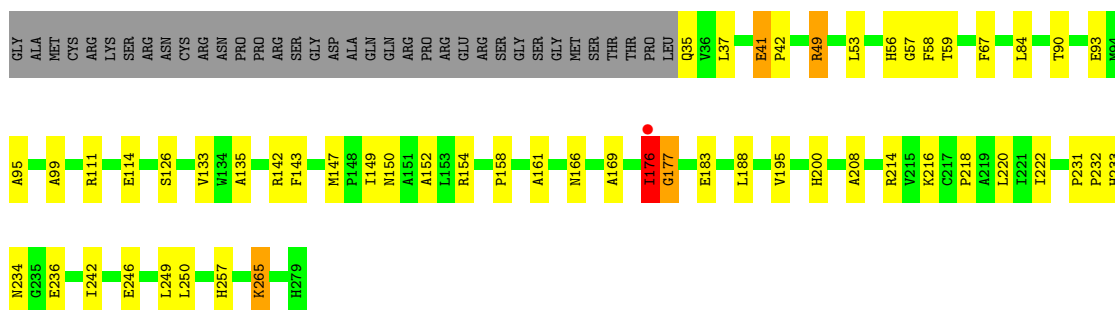
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	153	Total	O	0	0
			153	153		
4	B	164	Total	O	0	0
			164	164		
4	C	169	Total	O	0	0
			169	169		
4	D	122	Total	O	0	0
			122	122		

3 Residue-property plots

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.

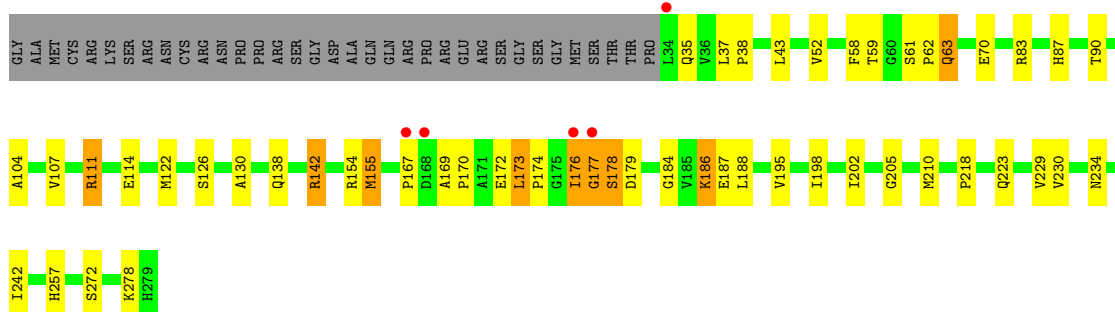
- Molecule 1: LipS lipolytic enzyme

Chain A: 



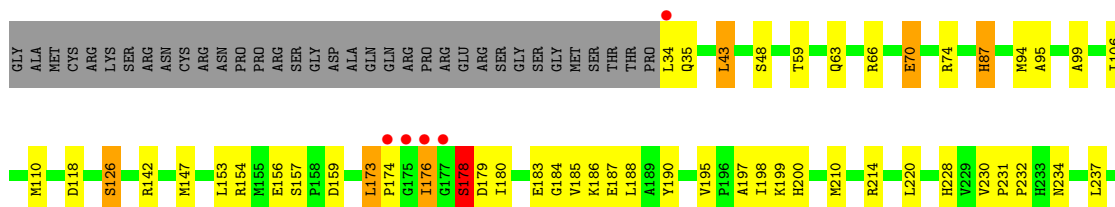
- Molecule 1: LipS lipolytic enzyme

Chain B: 



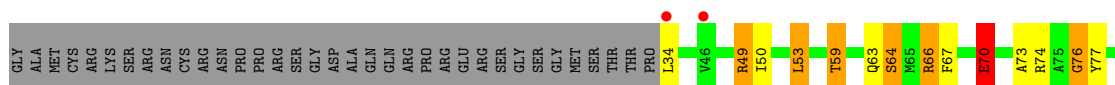
- Molecule 1: LipS lipolytic enzyme

Chain C: 





- Molecule 1: LipS lipolytic enzyme



4 Data and refinement statistics i

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 40.30 – 1.99	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.30-1.99) 100.0 (40.30-1.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.176 , 0.217 0.178 , 0.218	Depositor DCC
R_{free} test set	4535 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtrriage
Anisotropy	0.409	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.076 for h,-k,-l	Xtrriage
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

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 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: CL, SPD

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	1.70	12/1895 (0.6%)	1.34	9/2583 (0.3%)
1	B	1.61	13/1906 (0.7%)	1.32	10/2600 (0.4%)
1	C	1.69	15/1912 (0.8%)	1.39	16/2607 (0.6%)
1	D	1.55	10/1912 (0.5%)	1.33	15/2607 (0.6%)
All	All	1.64	50/7625 (0.7%)	1.35	50/10397 (0.5%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	ILE	CA-CB	8.60	1.65	1.54
1	D	152	ALA	CA-CB	7.47	1.64	1.53
1	B	90	THR	CA-CB	7.10	1.62	1.53
1	C	230	VAL	CA-CB	7.04	1.59	1.54
1	A	158	PRO	N-CA	6.64	1.56	1.47
1	C	273	LEU	N-CA	6.37	1.54	1.46
1	A	188	LEU	CA-C	6.17	1.60	1.52
1	D	70	GLU	N-CA	6.08	1.53	1.46
1	D	119	VAL	CA-CB	6.03	1.62	1.54
1	A	135	ALA	CA-CB	6.00	1.62	1.53
1	A	208	ALA	CA-CB	5.99	1.62	1.53
1	B	38	PRO	C-O	5.92	1.30	1.23
1	C	126	SER	C-O	-5.91	1.19	1.24
1	C	94	MET	CA-C	5.89	1.60	1.52
1	C	157	SER	CA-C	5.89	1.59	1.52
1	B	130	ALA	CA-CB	5.80	1.62	1.53
1	B	278	LYS	C-O	-5.78	1.16	1.24
1	C	153	LEU	N-CA	5.78	1.53	1.46
1	B	176	ILE	CA-CB	5.76	1.62	1.54
1	B	242	ILE	CA-CB	5.75	1.60	1.54
1	C	230	VAL	N-CA	-5.66	1.41	1.46
1	C	106	ILE	CA-CB	-5.64	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	VAL	CA-CB	5.63	1.57	1.53
1	D	157	SER	CA-C	5.56	1.59	1.52
1	A	133	VAL	CA-CB	-5.55	1.47	1.54
1	C	118	ASP	C-O	-5.54	1.17	1.24
1	B	223	GLN	N-CA	5.52	1.53	1.46
1	B	195	VAL	CA-CB	5.42	1.57	1.53
1	A	152	ALA	CA-C	5.41	1.58	1.53
1	C	199	LYS	CA-C	5.40	1.59	1.52
1	A	176	ILE	CA-C	5.39	1.59	1.52
1	C	95	ALA	CA-CB	5.38	1.62	1.53
1	C	176	ILE	CA-CB	5.37	1.61	1.54
1	B	210	MET	C-O	5.37	1.30	1.24
1	B	104	ALA	CA-CB	5.32	1.62	1.53
1	D	176	ILE	CA-CB	5.26	1.60	1.54
1	A	250	LEU	C-O	5.25	1.30	1.24
1	D	88	GLY	N-CA	5.23	1.52	1.45
1	A	95	ALA	C-O	-5.17	1.17	1.24
1	A	143	PHE	C-O	-5.14	1.17	1.24
1	D	107	VAL	CA-C	5.13	1.59	1.52
1	C	87	HIS	C-O	5.12	1.29	1.23
1	D	80	ALA	CA-CB	-5.10	1.45	1.53
1	B	83	ARG	CA-C	5.10	1.59	1.52
1	D	266	GLU	N-CA	5.10	1.52	1.46
1	B	205	GLY	C-O	5.08	1.29	1.23
1	D	59	THR	CA-CB	5.08	1.62	1.53
1	C	254	ASN	CA-C	-5.03	1.46	1.53
1	C	265	LYS	N-CA	5.02	1.52	1.46
1	B	122	MET	SD-CE	5.01	1.92	1.79

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	GLY	N-CA-C	9.02	122.25	112.33
1	A	242	ILE	CB-CA-C	-8.89	101.81	111.59
1	D	169	ALA	CA-C-N	-8.74	110.33	120.11
1	D	169	ALA	C-N-CA	-8.74	110.33	120.11
1	C	197	ALA	N-CA-C	-8.03	103.27	113.23
1	B	177	GLY	N-CA-C	7.48	120.11	111.36
1	D	204	ILE	CB-CA-C	-7.03	102.66	112.14
1	D	257	HIS	N-CA-C	6.98	118.54	111.07
1	A	265	LYS	CD-CE-NZ	-6.93	89.72	111.90
1	D	76	GLY	N-CA-C	6.91	124.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	SER	N-CA-C	6.80	121.03	111.92
1	A	90	THR	CA-C-N	6.64	126.43	119.05
1	A	90	THR	C-N-CA	6.64	126.43	119.05
1	B	37	LEU	CA-C-N	-6.63	113.13	119.76
1	B	37	LEU	C-N-CA	-6.63	113.13	119.76
1	C	242	ILE	CB-CA-C	-6.42	104.53	111.59
1	D	139	PHE	CA-C-N	-6.32	113.18	119.56
1	D	139	PHE	C-N-CA	-6.32	113.18	119.56
1	B	242	ILE	CB-CA-C	-6.11	104.61	111.45
1	C	173	LEU	CA-C-N	6.11	127.47	119.84
1	C	173	LEU	C-N-CA	6.11	127.47	119.84
1	C	126	SER	CB-CA-C	-6.06	108.99	117.23
1	B	173	LEU	CA-C-N	6.05	127.40	119.84
1	B	173	LEU	C-N-CA	6.05	127.40	119.84
1	C	198	ILE	N-CA-C	5.97	116.71	110.62
1	B	272	SER	N-CA-C	-5.93	104.39	111.69
1	D	147	MET	CA-C-N	-5.64	114.12	119.76
1	D	147	MET	C-N-CA	-5.64	114.12	119.76
1	C	70	GLU	CB-CA-C	-5.61	102.07	110.88
1	C	277	ARG	CB-CA-C	-5.61	100.26	110.63
1	A	111	ARG	CG-CD-NE	5.52	124.14	112.00
1	D	70	GLU	N-CA-CB	5.44	117.85	109.91
1	D	214	ARG	CB-CG-CD	-5.44	98.79	111.30
1	C	48	SER	N-CA-C	5.39	117.80	110.35
1	D	64	SER	N-CA-C	-5.39	105.96	112.54
1	D	159	ASP	N-CA-C	-5.37	105.43	111.28
1	C	195	VAL	CA-C-N	-5.32	114.13	119.56
1	C	195	VAL	C-N-CA	-5.32	114.13	119.56
1	B	52	VAL	CB-CA-C	-5.27	102.64	110.33
1	A	195	VAL	N-CA-CB	5.24	113.80	110.50
1	C	190	TYR	CA-C-N	5.21	125.67	120.04
1	C	190	TYR	C-N-CA	5.21	125.67	120.04
1	D	73	ALA	N-CA-C	-5.14	105.59	111.14
1	C	74	ARG	CG-CD-NE	-5.13	100.71	112.00
1	D	276	ILE	CB-CA-C	-5.13	105.40	111.97
1	A	37	LEU	CA-C-N	-5.12	114.30	119.83
1	A	37	LEU	C-N-CA	-5.12	114.30	119.83
1	C	214	ARG	NE-CZ-NH2	-5.11	114.60	119.20
1	B	198	ILE	N-CA-C	5.08	115.80	110.62
1	C	178	SER	N-CA-C	5.01	118.05	111.28

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	49	0
1	C	1867	0	1870	46	0
1	D	1867	0	1870	49	0
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	200	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 (200) 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:155:MET:HE3	1:B:155:MET:HA	1.28	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: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:155:MET:HA	1:B:155:MET:CE	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLY:N	2:A:301:SPD:C2	2.27	0.97
1:D:155:MET:HE1	1:D:230:VAL:HG22	1.47	0.96
1:B:111:ARG:HG3	1:B:111:ARG:HH11	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
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:B:59:THR:H	1:B:87:HIS:CE1	2.03	0.77
1:D:63:GLN:NE2	1:D:188:LEU:H	1.83	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:176:ILE:O	2:C:301:SPD:H22	1.87	0.74
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:110:MET:HE2	1:C:142:ARG:HH11	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C	2:A:301:SPD:H21	2.15	0.70
1:D:152:ALA:HB1	1:D:155:MET:HE3	1.72	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: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
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: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:D:225:ARG:HH21	1:D:253:GLU:CD	2.08	0.61
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:155:MET:HA	1:D:155:MET:HE2	1.86	0.57
1:D:49:ARG:HG3	1:D:118:ASP:OD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:110:MET:CE	1:C:142:ARG:HH11	2.18	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
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:C:43:LEU:HD12	1:C:43:LEU:C	2.33	0.54
1:A:41:GLU:H	1:A:41:GLU:CD	2.16	0.53
1:B:257:HIS:HD2	2:B:301:SPD:H32	1.73	0.53
1:C:242:ILE:HD12	1:C:244:SER:HB2	1.91	0.52
1:D:179:ASP:OD1	1:D:228:HIS:HD2	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:H92	2:C:301:SPD:C5	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:B:154:ARG:N	1:B:234:ASN:HD21	2.04	0.51
1:C:257:HIS:CD2	2:C:301:SPD:N10	2.78	0.51
1:B:155:MET:HE1	1:B:230:VAL:HA	1.93	0.51
1:B:59:THR:N	1:B:87:HIS:CE1	2.77	0.51
1:C:187:GLU:OE2	2:C:301:SPD:H71	2.09	0.51
1:A:126:SER:HG	2:A:301:SPD:H101	1.55	0.50
1:D:74:ARG:C	1:D:76:GLY:H	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:SPD:H72	4:C:441:HOH:O	2.10	0.49
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:B:61:SER:HB2	1:B:62:PRO:CD	2.44	0.47
1:D:215:VAL:HB	1:D:242:ILE:HG13	1.96	0.47
1:B:155:MET:HA	1:B:155:MET:HE2	1.89	0.47
1:C:159:ASP:OD1	4:C:464:HOH:O	2.21	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
1:B:155:MET:HE3	1:B:155:MET:CA	2.20	0.47
1:B:155:MET:HE1	1:B:230:VAL:HG22	1.97	0.46
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:147:MET:HA	1:C:220:LEU:O	2.15	0.45
1:C:179:ASP:OD1	1:C:228:HIS:CD2	2.63	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:HD12	1:D:204:ILE:HG23	1.72	0.45
2:A:301:SPD:H92	2:A:301:SPD:H41	1.98	0.45
1:B:178:SER:H	2:B:301:SPD:H21	1.82	0.45
1:B:43:LEU:HD11	1:B:70:GLU:HG3	2.00	0.44
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: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:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:SPD:H41	2:B:301:SPD:H71	1.31	0.43
1:C:63:GLN:HE21	1:C:188:LEU:H	1.64	0.43
1:A:161:ALA:HB2	1:C:210:MET:HB3	2.01	0.42
1:D:53:LEU:HB2	1:D:113:LEU:CD1	2.49	0.42
1:D:67:PHE:CZ	1:D:266:GLU:HG3	2.55	0.42
1:D:152:ALA:HB1	1:D:155:MET:CE	2.43	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:B:202:ILE:HG12	1:D:210:MET:HE1	2.02	0.42
1:C:178:SER:N	2:C:301:SPD:H21	2.34	0.42
1:B:138:GLN:NE2	4:B:415:HOH:O	2.53	0.42
1:D:59:THR:N	1:D:87:HIS:CE1	2.86	0.42
1:D:63:GLN:NE2	1:D:187:GLU:HA	2.35	0.42
1:A:214:ARG:HD2	4:C:464:HOH:O	2.20	0.41
1:A:58:PHE:HB3	3:A:302:CL:CL	2.57	0.41
1:A:126:SER:HA	1:A:150:ASN:O	2.19	0.41
1:B:58:PHE:HB3	3:B:302:CL:CL	2.57	0.41
1:D:110:MET:HE1	1:D:139:PHE:CD2	2.56	0.41
1:A:149:ILE:HA	1:A:222:ILE:O	2.20	0.41
1:C:66:ARG:NH1	1:C:66:ARG:HG3	2.36	0.41
1:A:218:PRO:HB3	1:A:246:GLU:HG2	2.02	0.41
1:A:231:PRO:HA	1:A:232:PRO:HD3	1.94	0.41
2:A:301:SPD:H92	2:A:301:SPD:C5	2.51	0.41
1:A:176:ILE:HD13	1:A:176:ILE:HG21	1.71	0.41
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 [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	243/281 (86%)	232 (96%)	11 (4%)	0	100	100
1	B	245/281 (87%)	235 (96%)	9 (4%)	1 (0%)	30	27
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%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/223 (86%)	185 (96%)	8 (4%)	27	26
1	B	194/223 (87%)	188 (97%)	6 (3%)	35	37
1	C	195/223 (87%)	185 (95%)	10 (5%)	21	19
1	D	195/223 (87%)	185 (95%)	10 (5%)	21	19
All	All	777/892 (87%)	743 (96%)	34 (4%)	25	24

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	216	LYS
1	A	249	LEU
1	B	63	GLN
1	B	111	ARG

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Mol	Chain	Res	Type
1	B	142	ARG
1	B	155	MET
1	B	186	LYS
1	B	218	PRO
1	C	34	LEU
1	C	43	LEU
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
1	C	278	LYS
1	D	34	LEU
1	D	49	ARG
1	D	53	LEU
1	D	66	ARG
1	D	70	GLU
1	D	116	ARG
1	D	120	LEU
1	D	142	ARG
1	D	216	LYS
1	D	261	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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	B	87	HIS
1	B	200	HIS
1	B	233	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

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Mol	Chain	Res	Type
1	D	87	HIS
1	D	200	HIS
1	D	223	GLN
1	D	228	HIS
1	D	234	ASN

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 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	B	301	-	9,9,9	0.50	0	8,8,8	1.75	2 (25%)
2	SPD	A	301	-	9,9,9	0.80	0	8,8,8	1.38	2 (25%)
2	SPD	C	301	-	9,9,9	0.65	0	8,8,8	1.08	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	B	301	-	-	5/7/7/7	-
2	SPD	A	301	-	-	6/7/7/7	-
2	SPD	C	301	-	-	5/7/7/7	-

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	-3.26	103.32	112.07
2	B	301	SPD	C8-C7-N6	-2.70	104.82	112.07
2	A	301	SPD	C7-N6-C5	2.44	124.93	113.40
2	C	301	SPD	C4-C5-N6	-2.23	106.08	112.07
2	A	301	SPD	C3-C2-N1	2.05	126.75	112.60

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	SPD	C4-C5-N6-C7
2	B	301	SPD	C4-C5-N6-C7
2	C	301	SPD	C4-C5-N6-C7
2	C	301	SPD	N6-C7-C8-C9
2	B	301	SPD	C3-C4-C5-N6
2	C	301	SPD	C3-C4-C5-N6
2	B	301	SPD	C2-C3-C4-C5
2	A	301	SPD	N6-C7-C8-C9
2	A	301	SPD	C2-C3-C4-C5
2	A	301	SPD	C7-C8-C9-N10
2	B	301	SPD	C8-C7-N6-C5
2	C	301	SPD	C2-C3-C4-C5
2	B	301	SPD	C7-C8-C9-N10
2	C	301	SPD	C7-C8-C9-N10
2	A	301	SPD	N1-C2-C3-C4
2	A	301	SPD	C8-C7-N6-C5

There are no ring outliers.

3 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	SPD	14	0
2	A	301	SPD	21	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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%)	-0.40	1 (0%) 88 88	12, 23, 37, 50	0
1	B	246/281 (87%)	-0.31	5 (2%) 65 64	14, 24, 46, 58	1 (0%)
1	C	246/281 (87%)	-0.35	5 (2%) 65 64	14, 24, 39, 52	1 (0%)
1	D	246/281 (87%)	0.20	7 (2%) 55 54	17, 34, 50, 59	1 (0%)
All	All	983/1124 (87%)	-0.21	18 (1%) 67 67	12, 26, 46, 59	3 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	176	ILE	4.7
1	B	176	ILE	4.0
1	C	176	ILE	3.7
1	B	34	LEU	3.3
1	A	176	ILE	3.2
1	B	177	GLY	2.7
1	C	34	LEU	2.5
1	C	177	GLY	2.4
1	C	175	GLY	2.3
1	D	34	LEU	2.3
1	D	279	HIS	2.2
1	C	174	PRO	2.2
1	D	175	GLY	2.2
1	D	177	GLY	2.2
1	D	278	LYS	2.1
1	B	168	ASP	2.1
1	B	167	PRO	2.1
1	D	46	VAL	2.1

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(Å ²)	Q<0.9
2	SPD	A	301	10/10	0.84	0.17	25,43,50,52	0
2	SPD	C	301	10/10	0.85	0.15	30,41,48,49	0
2	SPD	B	301	10/10	0.87	0.13	32,37,44,47	0
3	CL	C	302	1/1	0.98	0.07	34,34,34,34	0
3	CL	D	301	1/1	0.98	0.09	33,33,33,33	0
3	CL	A	302	1/1	0.99	0.05	29,29,29,29	0
3	CL	B	302	1/1	0.99	0.06	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.