



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:35 am GMT

PDB ID : 5DIR
Title : membrane protein at 2.8 Angstroms
Authors : Vogeley, L.; El Arnaout, T.; Bailey, J.; Boland, C.; Caffrey, M.
Deposited on : 2015-09-01
Resolution : 2.80 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

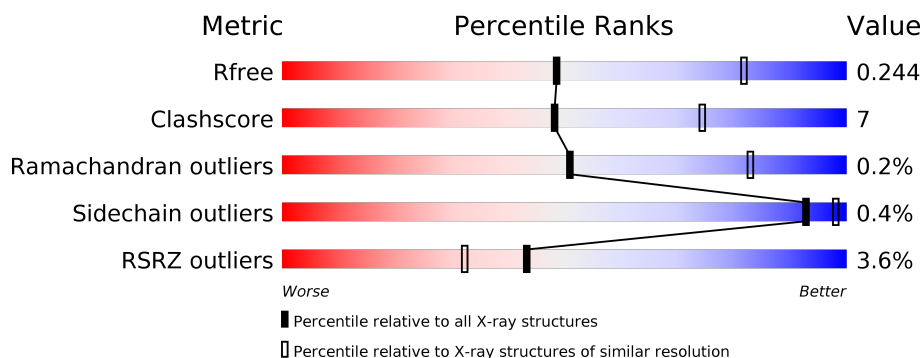
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	188	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>11%</div> <div>16%</div> </div> </div>
1	B	188	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>14%</div> <div>21%</div> </div> </div>
1	C	188	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>10%</div> <div>21%</div> </div> </div>
1	D	188	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>9%</div> <div>21%</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ALO	C	204	-	-	-	X
7	OLC	A	206	-	-	-	X
7	OLC	A	207	-	-	-	X
7	OLC	A	209	-	-	-	X
7	OLC	A	210	-	-	-	X
7	OLC	A	211	-	-	-	X
7	OLC	B	206	-	-	-	X
7	OLC	B	207	-	-	-	X
7	OLC	B	209	-	-	-	X
7	OLC	B	210	-	-	-	X
7	OLC	B	211	-	-	-	X
7	OLC	B	212	-	-	-	X
7	OLC	C	206	-	-	-	X
7	OLC	C	207	-	-	-	X
7	OLC	C	209	-	-	-	X
7	OLC	C	210	-	-	-	X
7	OLC	C	211	-	-	-	X
7	OLC	D	206	-	-	-	X
7	OLC	D	207	-	-	-	X
7	OLC	D	209	-	-	-	X
7	OLC	D	210	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5653 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 Lipoprotein signal peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1261	848	202	207	4			
1	B	149	Total	C	N	O	S	0	0	0
			1198	806	194	195	3			
1	C	149	Total	C	N	O	S	0	0	0
			1197	807	191	195	4			
1	D	149	Total	C	N	O	S	0	0	0
			1197	807	191	195	4			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP Q9HVM5
A	-17	SER	-	expression tag	UNP Q9HVM5
A	-16	SER	-	expression tag	UNP Q9HVM5
A	-15	HIS	-	expression tag	UNP Q9HVM5
A	-14	HIS	-	expression tag	UNP Q9HVM5
A	-13	HIS	-	expression tag	UNP Q9HVM5
A	-12	HIS	-	expression tag	UNP Q9HVM5
A	-11	HIS	-	expression tag	UNP Q9HVM5
A	-10	HIS	-	expression tag	UNP Q9HVM5
A	-9	SER	-	expression tag	UNP Q9HVM5
A	-8	SER	-	expression tag	UNP Q9HVM5
A	-7	GLY	-	expression tag	UNP Q9HVM5
A	-6	LEU	-	expression tag	UNP Q9HVM5
A	-5	VAL	-	expression tag	UNP Q9HVM5
A	-4	PRO	-	expression tag	UNP Q9HVM5
A	-3	ARG	-	expression tag	UNP Q9HVM5
A	-2	GLY	-	expression tag	UNP Q9HVM5
A	-1	SER	-	expression tag	UNP Q9HVM5
A	0	HIS	-	expression tag	UNP Q9HVM5
B	-18	GLY	-	expression tag	UNP Q9HVM5
B	-17	SER	-	expression tag	UNP Q9HVM5

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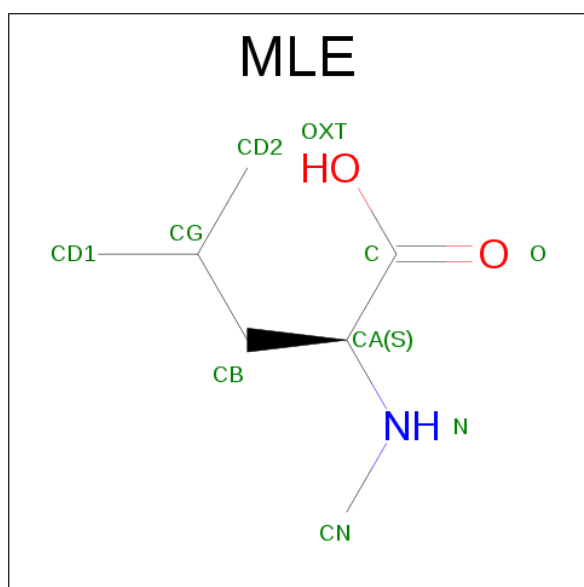
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP Q9HVM5
B	-15	HIS	-	expression tag	UNP Q9HVM5
B	-14	HIS	-	expression tag	UNP Q9HVM5
B	-13	HIS	-	expression tag	UNP Q9HVM5
B	-12	HIS	-	expression tag	UNP Q9HVM5
B	-11	HIS	-	expression tag	UNP Q9HVM5
B	-10	HIS	-	expression tag	UNP Q9HVM5
B	-9	SER	-	expression tag	UNP Q9HVM5
B	-8	SER	-	expression tag	UNP Q9HVM5
B	-7	GLY	-	expression tag	UNP Q9HVM5
B	-6	LEU	-	expression tag	UNP Q9HVM5
B	-5	VAL	-	expression tag	UNP Q9HVM5
B	-4	PRO	-	expression tag	UNP Q9HVM5
B	-3	ARG	-	expression tag	UNP Q9HVM5
B	-2	GLY	-	expression tag	UNP Q9HVM5
B	-1	SER	-	expression tag	UNP Q9HVM5
B	0	HIS	-	expression tag	UNP Q9HVM5
C	-18	GLY	-	expression tag	UNP Q9HVM5
C	-17	SER	-	expression tag	UNP Q9HVM5
C	-16	SER	-	expression tag	UNP Q9HVM5
C	-15	HIS	-	expression tag	UNP Q9HVM5
C	-14	HIS	-	expression tag	UNP Q9HVM5
C	-13	HIS	-	expression tag	UNP Q9HVM5
C	-12	HIS	-	expression tag	UNP Q9HVM5
C	-11	HIS	-	expression tag	UNP Q9HVM5
C	-10	HIS	-	expression tag	UNP Q9HVM5
C	-9	SER	-	expression tag	UNP Q9HVM5
C	-8	SER	-	expression tag	UNP Q9HVM5
C	-7	GLY	-	expression tag	UNP Q9HVM5
C	-6	LEU	-	expression tag	UNP Q9HVM5
C	-5	VAL	-	expression tag	UNP Q9HVM5
C	-4	PRO	-	expression tag	UNP Q9HVM5
C	-3	ARG	-	expression tag	UNP Q9HVM5
C	-2	GLY	-	expression tag	UNP Q9HVM5
C	-1	SER	-	expression tag	UNP Q9HVM5
C	0	HIS	-	expression tag	UNP Q9HVM5
D	-18	GLY	-	expression tag	UNP Q9HVM5
D	-17	SER	-	expression tag	UNP Q9HVM5
D	-16	SER	-	expression tag	UNP Q9HVM5
D	-15	HIS	-	expression tag	UNP Q9HVM5
D	-14	HIS	-	expression tag	UNP Q9HVM5
D	-13	HIS	-	expression tag	UNP Q9HVM5

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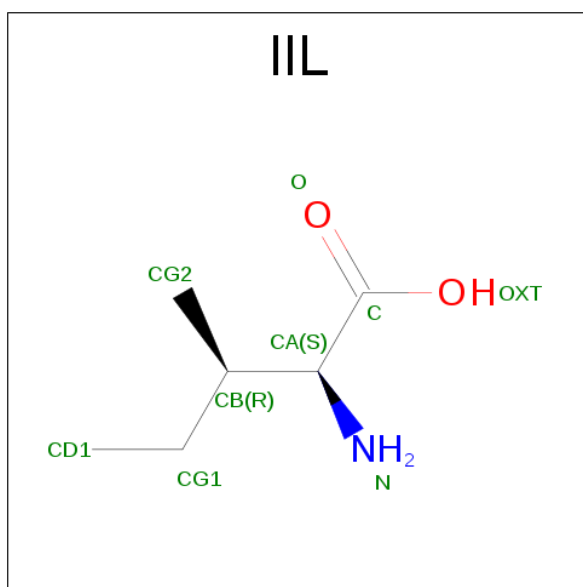
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP Q9HVM5
D	-11	HIS	-	expression tag	UNP Q9HVM5
D	-10	HIS	-	expression tag	UNP Q9HVM5
D	-9	SER	-	expression tag	UNP Q9HVM5
D	-8	SER	-	expression tag	UNP Q9HVM5
D	-7	GLY	-	expression tag	UNP Q9HVM5
D	-6	LEU	-	expression tag	UNP Q9HVM5
D	-5	VAL	-	expression tag	UNP Q9HVM5
D	-4	PRO	-	expression tag	UNP Q9HVM5
D	-3	ARG	-	expression tag	UNP Q9HVM5
D	-2	GLY	-	expression tag	UNP Q9HVM5
D	-1	SER	-	expression tag	UNP Q9HVM5
D	0	HIS	-	expression tag	UNP Q9HVM5

- Molecule 2 is N-METHYLLEUCINE (three-letter code: MLE) (formula: $C_7H_{15}NO_2$).



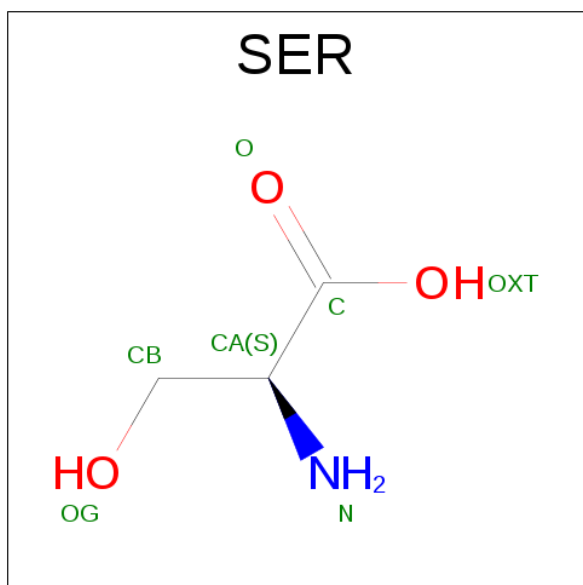
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	7	1	1		
2	B	1	Total	C	N	O	0	0
			9	7	1	1		
2	C	1	Total	C	N	O	0	0
			9	7	1	1		
2	D	1	Total	C	N	O	0	0
			9	7	1	1		

- Molecule 3 is ISO-ISOLEUCINE (three-letter code: IIL) (formula: $C_6H_{13}NO_2$).



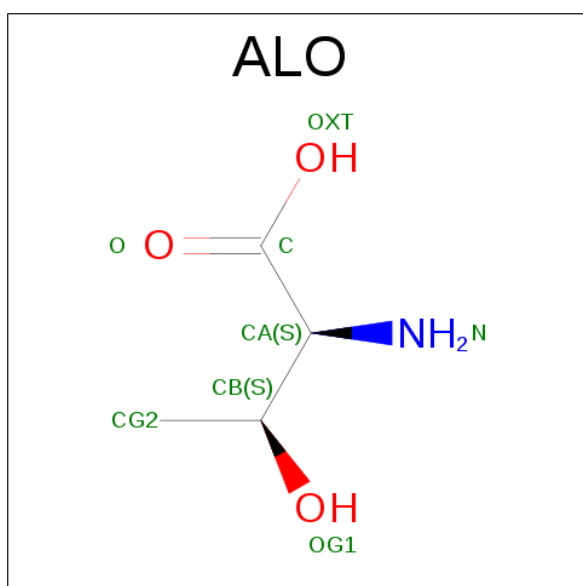
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	6	1	1		
3	B	1	Total	C	N	O	0	0
			8	6	1	1		
3	C	1	Total	C	N	O	0	0
			8	6	1	1		
3	D	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 4 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



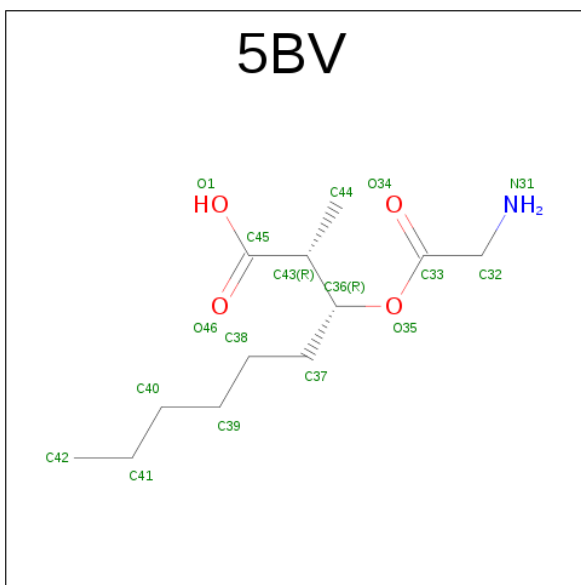
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			6	3	1	2		
4	B	1	Total	C	N	O	0	0
			6	3	1	2		
4	C	1	Total	C	N	O	0	0
			6	3	1	2		
4	D	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 5 is ALLO-THREONINE (three-letter code: ALO) (formula: $C_4H_9NO_3$).



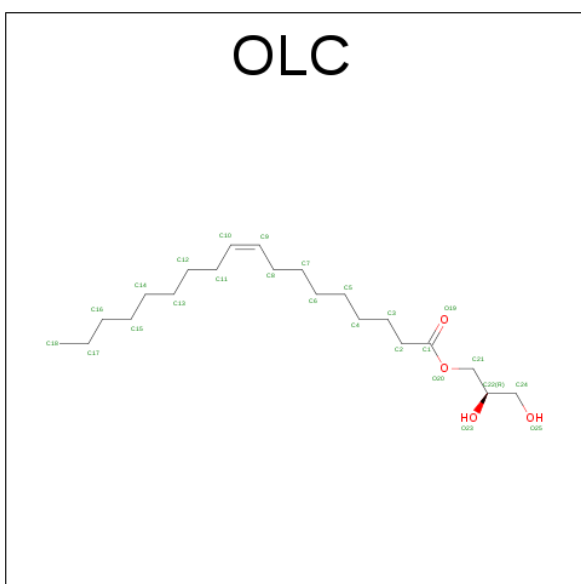
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			7	4	1	2		
5	B	1	Total	C	N	O	0	0
			7	4	1	2		
5	C	1	Total	C	N	O	0	0
			7	4	1	2		
5	D	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 6 is (2R,3R)-3-(glycyloxy)-2-methylnonanoic acid (three-letter code: 5BV) (formula: $C_{12}H_{23}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			16	12	1	3		
6	B	1	Total	C	N	O	0	0
			16	12	1	3		
6	C	1	Total	C	N	O	0	0
			16	12	1	3		
6	D	1	Total	C	N	O	0	0
			16	12	1	3		

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			25	21	4		
7	A	1	Total	C	O	0	0
			25	21	4		
7	A	1	Total	C	O	0	0
			25	21	4		
7	A	1	Total	C	O	0	0
			25	21	4		
7	A	1	Total	C	O	0	0
			25	21	4		
7	B	1	Total	C	O	0	0
			25	21	4		
7	B	1	Total	C	O	0	0
			25	21	4		
7	B	1	Total	C	O	0	0
			25	21	4		
7	B	1	Total	C	O	0	0
			25	21	4		
7	B	1	Total	C	O	0	0
			25	21	4		
7	B	1	Total	C	O	0	0
			25	21	4		
7	C	1	Total	C	O	0	0
			25	21	4		
7	C	1	Total	C	O	0	0
			25	21	4		
7	C	1	Total	C	O	0	0
			25	21	4		
7	C	1	Total	C	O	0	0
			25	21	4		
7	C	1	Total	C	O	0	0
			25	21	4		
7	C	1	Total	C	O	0	0
			25	21	4		
7	D	1	Total	C	O	0	0
			25	21	4		
7	D	1	Total	C	O	0	0
			25	21	4		
7	D	1	Total	C	O	0	0
			25	21	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			25	21	4		
7	D	1	Total	C	O	0	0
			25	21	4		

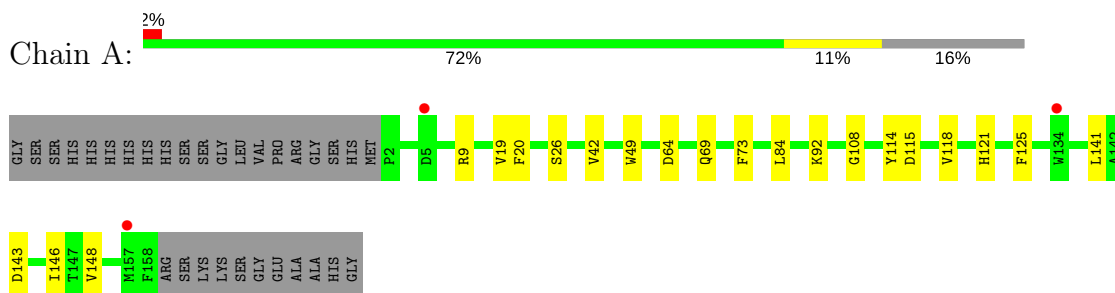
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	O	0	0
			4	4		
8	B	2	Total	O	0	0
			2	2		
8	C	6	Total	O	0	0
			6	6		
8	D	4	Total	O	0	0
			4	4		

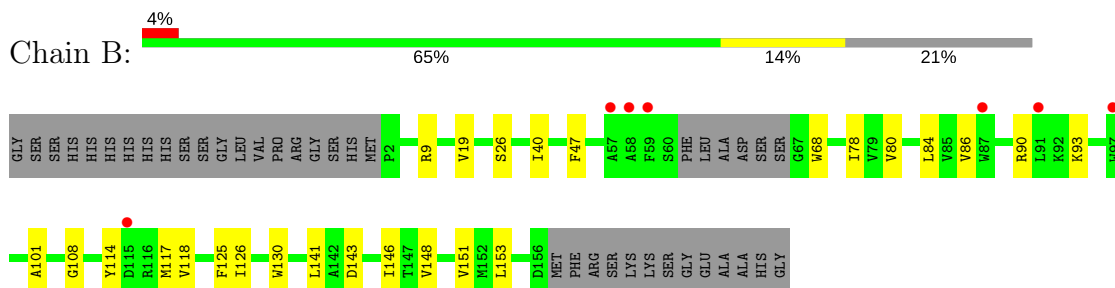
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

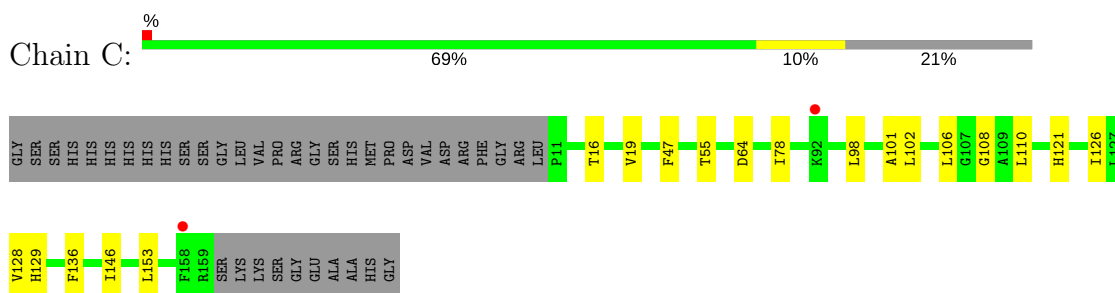
- Molecule 1: Lipoprotein signal peptidase



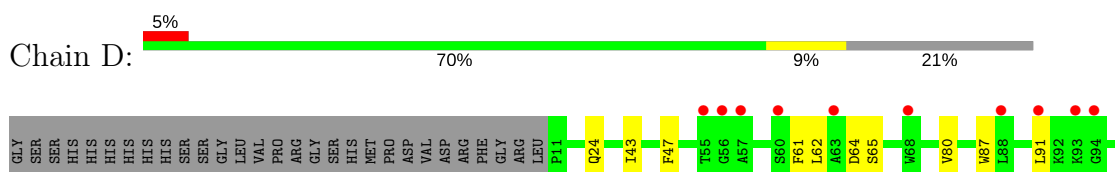
- Molecule 1: Lipoprotein signal peptidase



- Molecule 1: Lipoprotein signal peptidase



- Molecule 1: Lipoprotein signal peptidase



G111	
V122	
F125	
I126	
L141	
A142	
D143	
V148	
R189	
SER	
LYS	
LYS	
SER	
GLY	
GLU	
ALA	
ALA	
HIS	
GLY	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.48Å 105.88Å 85.39Å 90.00° 96.92° 90.00°	Depositor
Resolution (Å)	44.90 – 2.80 44.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (44.90-2.80) 97.6 (44.90-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1894)	Depositor
R, R_{free}	0.219 , 0.245 0.218 , 0.244	Depositor DCC
R_{free} test set	1208 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5653	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.28% 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: ALO, 5BV, OLC, IIL, MLE

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	0.26	0/1300	0.46	0/1777
1	B	0.27	0/1234	0.49	0/1687
1	C	0.27	0/1234	0.49	0/1687
1	D	0.26	0/1234	0.48	0/1687
All	All	0.27	0/5002	0.48	0/6838

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1261	0	1273	15	0
1	B	1198	0	1215	20	0
1	C	1197	0	1213	13	0
1	D	1197	0	1213	14	0
2	A	9	0	13	1	0
2	B	9	0	13	0	0
2	C	9	0	13	0	0
2	D	9	0	13	1	0
3	A	8	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	10	0	0
3	C	8	0	10	0	0
3	D	8	0	10	0	0
4	A	6	0	5	0	0
4	B	6	0	5	1	0
4	C	6	0	5	0	0
4	D	6	0	5	2	0
5	A	7	0	7	0	0
5	B	7	0	7	0	0
5	C	7	0	7	0	0
5	D	7	0	7	0	0
6	A	16	0	0	1	0
6	B	16	0	0	0	0
6	C	16	0	0	0	0
6	D	16	0	0	0	0
7	A	150	0	240	14	0
7	B	175	0	280	9	0
7	C	150	0	240	11	0
7	D	125	0	200	6	0
8	A	4	0	0	0	0
8	B	2	0	0	0	0
8	C	6	0	0	1	0
8	D	4	0	0	0	0
All	All	5653	0	6014	80	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 7.

All (80) 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:B:148:VAL:HG11	7:B:206:OLC:H13A	1.69	0.72
1:A:49:TRP:HE1	7:A:208:OLC:H4A	1.56	0.70
1:A:148:VAL:HG21	7:A:206:OLC:H12A	1.76	0.67
7:A:207:OLC:H18A	7:A:208:OLC:H15A	1.79	0.64
1:C:129:HIS:NE2	8:C:301:HOH:O	2.30	0.64
1:B:148:VAL:HG21	7:B:206:OLC:H11	1.82	0.61
1:B:78:ILE:HD11	1:B:117:MET:HE3	1.83	0.59
1:D:143:ASP:OD2	4:D:203:SER:OG	2.19	0.59
7:C:209:OLC:H18A	7:C:210:OLC:H18A	1.85	0.58
1:A:108:GLY:HA3	1:A:146:ILE:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:PHE:HE2	7:A:210:OLC:H17A	1.70	0.57
7:A:206:OLC:H17	7:A:209:OLC:H12A	1.88	0.56
1:C:19:VAL:HG22	7:C:206:OLC:H17A	1.88	0.56
1:C:110:LEU:HB3	7:C:209:OLC:H10	1.88	0.55
1:D:80:VAL:HG11	2:D:201:MLE:HD21	1.89	0.55
1:D:148:VAL:HG21	7:D:206:OLC:H11A	1.89	0.55
1:C:101:ALA:HB1	1:C:153:LEU:HD12	1.89	0.54
1:C:47:PHE:HE1	1:C:126:ILE:HG23	1.73	0.53
1:B:47:PHE:HE1	1:B:126:ILE:HG23	1.74	0.53
1:B:130:TRP:CD2	7:B:211:OLC:H3A	2.44	0.53
1:A:19:VAL:HG22	7:A:209:OLC:H16	1.91	0.52
1:B:143:ASP:OD2	4:B:203:SER:OG	2.28	0.51
1:D:141:LEU:HD21	7:D:207:OLC:H12	1.93	0.50
1:C:16:THR:HG21	1:C:106:LEU:HD22	1.93	0.50
1:A:143:ASP:HB3	7:A:206:OLC:H21A	1.93	0.50
1:B:108:GLY:HA3	1:B:146:ILE:HG13	1.94	0.50
1:A:42:VAL:HG22	7:A:208:OLC:H2A	1.93	0.50
1:B:151:VAL:HG12	7:B:207:OLC:H7A	1.94	0.50
1:D:47:PHE:HE1	1:D:126:ILE:HG23	1.77	0.49
1:B:101:ALA:HB1	1:B:153:LEU:HD12	1.95	0.49
1:A:141:LEU:HD21	7:A:207:OLC:H14A	1.94	0.49
1:D:122:VAL:HG11	4:D:203:SER:HB3	1.93	0.49
1:B:26:SER:HB3	1:B:125:PHE:CZ	2.48	0.49
1:D:43:ILE:HD11	7:D:210:OLC:H15	1.95	0.48
1:C:55:THR:HG22	1:C:121:HIS:HB3	1.95	0.48
1:D:24:GLN:NE2	1:D:111:GLY:O	2.47	0.48
1:C:128:VAL:HG23	1:C:136:PHE:HB3	1.96	0.47
1:B:9:ARG:CZ	1:B:93:LYS:HG3	2.45	0.47
7:A:206:OLC:H8A	7:A:206:OLC:H11	1.66	0.46
1:B:148:VAL:O	1:B:151:VAL:HG22	2.15	0.46
1:A:26:SER:HB3	1:A:125:PHE:CZ	2.50	0.46
1:B:40:ILE:HD13	7:B:212:OLC:H21A	1.97	0.46
1:D:125:PHE:HZ	1:D:141:LEU:HD13	1.81	0.46
1:B:114:TYR:CE1	1:B:118:VAL:HG21	2.51	0.46
7:D:208:OLC:H11	7:D:208:OLC:H8A	1.43	0.45
7:D:207:OLC:H11	7:D:207:OLC:H8	1.43	0.45
1:C:108:GLY:HA3	1:C:146:ILE:HG13	1.99	0.45
7:A:207:OLC:H11A	7:A:207:OLC:H8	1.46	0.45
1:A:69:GLN:HB3	1:A:73:PHE:CE2	2.52	0.45
7:A:210:OLC:H8	7:A:210:OLC:H11	1.75	0.45
1:A:9:ARG:HH21	1:A:92:LYS:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:210:OLC:H11A	7:C:210:OLC:H8	1.76	0.44
1:D:87:TRP:O	1:D:91:LEU:HD13	2.16	0.44
7:B:212:OLC:H11A	7:B:212:OLC:H8	1.39	0.44
7:C:209:OLC:H11	7:C:209:OLC:H8	1.49	0.44
1:A:114:TYR:CZ	1:A:118:VAL:HG21	2.52	0.44
7:C:208:OLC:H16	7:C:211:OLC:H17A	1.99	0.43
7:C:210:OLC:H12	7:C:210:OLC:H15	1.62	0.43
1:B:86:VAL:O	1:B:90:ARG:HG2	2.19	0.43
7:C:208:OLC:H11	7:C:208:OLC:H8	1.55	0.43
1:A:84:LEU:HD12	1:A:84:LEU:HA	1.86	0.43
7:A:209:OLC:H8A	7:A:209:OLC:H11	1.72	0.43
1:B:68:TRP:CH2	1:D:62:LEU:HD22	2.54	0.43
1:B:141:LEU:HA	1:B:141:LEU:HD23	1.84	0.42
1:B:19:VAL:HG22	7:B:209:OLC:H16	2.01	0.42
7:C:208:OLC:H14	7:C:211:OLC:H15A	2.01	0.42
1:B:68:TRP:NE1	1:D:65:SER:OG	2.52	0.42
1:D:64:ASP:OD1	1:D:64:ASP:N	2.52	0.42
7:B:208:OLC:H11A	7:B:208:OLC:H8	1.67	0.42
1:A:115:ASP:HB3	1:A:121:HIS:O	2.20	0.42
1:D:143:ASP:HB3	7:D:206:OLC:H21A	2.02	0.42
1:C:110:LEU:HD13	7:C:209:OLC:H10	2.02	0.41
2:A:201:MLE:HG	6:A:205:5BV:C45	2.49	0.41
3:A:202:IIL:HD12	7:A:206:OLC:H21	2.03	0.41
7:B:209:OLC:H9	7:B:209:OLC:H6	1.72	0.41
1:C:78:ILE:HG12	7:C:210:OLC:H10	2.01	0.41
1:B:80:VAL:O	1:B:84:LEU:HD13	2.21	0.41
1:C:98:LEU:O	1:C:102:LEU:HD13	2.21	0.40
1:A:64:ASP:N	1:A:64:ASP:OD1	2.54	0.40
1:C:64:ASP:OD1	1:C:64:ASP:N	2.52	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	155/188 (82%)	153 (99%)	2 (1%)	0	100	100
1	B	145/188 (77%)	143 (99%)	2 (1%)	0	100	100
1	C	147/188 (78%)	140 (95%)	7 (5%)	0	100	100
1	D	147/188 (78%)	142 (97%)	4 (3%)	1 (1%)	25	59
All	All	594/752 (79%)	578 (97%)	15 (2%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	61	PHE

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	130/154 (84%)	130 (100%)	0	100	100
1	B	123/154 (80%)	123 (100%)	0	100	100
1	C	123/154 (80%)	123 (100%)	0	100	100
1	D	123/154 (80%)	123 (100%)	0	100	100
All	All	499/616 (81%)	499 (100%)	0	93	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

44 ligands 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	MLE	A	201	3,6	8,8,9	1.21	1 (12%)	7,9,11	1.32	1 (14%)
3	IIL	A	202	2,4	7,7,8	1.20	1 (14%)	6,8,10	1.01	0
4	SER	A	203	3,5	5,5,6	1.19	1 (20%)	1,5,7	1.91	0
5	ALO	A	204	4,6	6,6,7	0.91	0	6,7,9	0.90	0
6	5BV	A	205	2,5	14,15,16	0.47	0	14,17,19	1.03	1 (7%)
7	OLC	A	206	-	24,24,24	0.54	0	25,25,25	0.92	0
7	OLC	A	207	-	24,24,24	0.51	0	25,25,25	0.82	0
7	OLC	A	208	-	24,24,24	0.49	0	25,25,25	0.87	0
7	OLC	A	209	-	24,24,24	0.51	0	25,25,25	0.77	0
7	OLC	A	210	-	24,24,24	0.53	0	25,25,25	0.77	0
7	OLC	A	211	-	24,24,24	0.51	0	25,25,25	0.81	0
2	MLE	B	201	3,6	8,8,9	1.25	1 (12%)	7,9,11	1.13	1 (14%)
3	IIL	B	202	2,4	7,7,8	1.23	1 (14%)	6,8,10	0.97	0
4	SER	B	203	3,5	5,5,6	1.33	1 (20%)	1,5,7	1.79	0
5	ALO	B	204	4,6	6,6,7	0.90	0	6,7,9	0.73	0
6	5BV	B	205	2,5	14,15,16	0.42	0	14,17,19	1.11	0
7	OLC	B	206	-	24,24,24	0.52	0	25,25,25	0.81	0
7	OLC	B	207	-	24,24,24	0.51	0	25,25,25	0.85	0
7	OLC	B	208	-	24,24,24	0.47	0	25,25,25	0.92	0
7	OLC	B	209	-	24,24,24	0.52	0	25,25,25	0.95	0
7	OLC	B	210	-	24,24,24	0.52	0	25,25,25	0.79	0
7	OLC	B	211	-	24,24,24	0.54	0	25,25,25	0.73	0
7	OLC	B	212	-	24,24,24	0.51	0	25,25,25	0.81	0
2	MLE	C	201	3,6	8,8,9	1.22	1 (12%)	7,9,11	1.25	1 (14%)
3	IIL	C	202	2,4	7,7,8	1.24	1 (14%)	6,8,10	1.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SER	C	203	3,5	5,5,6	1.16	1 (20%)	1,5,7	1.91	0
5	ALO	C	204	4,6	6,6,7	0.96	1 (16%)	6,7,9	0.76	0
6	5BV	C	205	2,5	14,15,16	0.44	0	14,17,19	0.97	1 (7%)
7	OLC	C	206	-	24,24,24	0.52	0	25,25,25	0.79	0
7	OLC	C	207	-	24,24,24	0.49	0	25,25,25	0.84	0
7	OLC	C	208	-	24,24,24	0.51	0	25,25,25	0.83	0
7	OLC	C	209	-	24,24,24	0.50	0	25,25,25	0.82	0
7	OLC	C	210	-	24,24,24	0.54	0	25,25,25	0.73	0
7	OLC	C	211	-	24,24,24	0.52	0	25,25,25	0.87	0
2	MLE	D	201	3,6	8,8,9	1.13	1 (12%)	7,9,11	1.16	1 (14%)
3	IIL	D	202	2,4	7,7,8	1.15	1 (14%)	6,8,10	1.07	0
4	SER	D	203	3,5	5,5,6	1.17	1 (20%)	1,5,7	1.55	0
5	ALO	D	204	4,6	6,6,7	1.12	1 (16%)	6,7,9	0.80	0
6	5BV	D	205	2,5	14,15,16	0.42	0	14,17,19	0.97	1 (7%)
7	OLC	D	206	-	24,24,24	0.53	0	25,25,25	0.74	0
7	OLC	D	207	-	24,24,24	0.53	0	25,25,25	0.81	0
7	OLC	D	208	-	24,24,24	0.52	0	25,25,25	0.78	0
7	OLC	D	209	-	24,24,24	0.54	0	25,25,25	0.80	0
7	OLC	D	210	-	24,24,24	0.56	0	25,25,25	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	MLE	A	201	3,6	-	0/4/8/10	0/0/0/0
3	IIL	A	202	2,4	-	0/7/8/10	0/0/0/0
4	SER	A	203	3,5	-	0/2/4/6	0/0/0/0
5	ALO	A	204	4,6	-	0/4/6/8	0/0/0/0
6	5BV	A	205	2,5	-	0/17/18/20	0/0/0/0
7	OLC	A	206	-	-	0/24/24/24	0/0/0/0
7	OLC	A	207	-	-	0/24/24/24	0/0/0/0
7	OLC	A	208	-	-	0/24/24/24	0/0/0/0
7	OLC	A	209	-	-	0/24/24/24	0/0/0/0
7	OLC	A	210	-	-	0/24/24/24	0/0/0/0
7	OLC	A	211	-	-	0/24/24/24	0/0/0/0
2	MLE	B	201	3,6	-	0/4/8/10	0/0/0/0
3	IIL	B	202	2,4	-	0/7/8/10	0/0/0/0
4	SER	B	203	3,5	-	0/2/4/6	0/0/0/0
5	ALO	B	204	4,6	-	0/4/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5BV	B	205	2,5	-	0/17/18/20	0/0/0/0
7	OLC	B	206	-	-	0/24/24/24	0/0/0/0
7	OLC	B	207	-	-	0/24/24/24	0/0/0/0
7	OLC	B	208	-	-	0/24/24/24	0/0/0/0
7	OLC	B	209	-	-	0/24/24/24	0/0/0/0
7	OLC	B	210	-	-	0/24/24/24	0/0/0/0
7	OLC	B	211	-	-	0/24/24/24	0/0/0/0
7	OLC	B	212	-	-	0/24/24/24	0/0/0/0
2	MLE	C	201	3,6	-	0/4/8/10	0/0/0/0
3	IIL	C	202	2,4	-	0/7/8/10	0/0/0/0
4	SER	C	203	3,5	-	0/2/4/6	0/0/0/0
5	ALO	C	204	4,6	-	0/4/6/8	0/0/0/0
6	5BV	C	205	2,5	-	0/17/18/20	0/0/0/0
7	OLC	C	206	-	-	0/24/24/24	0/0/0/0
7	OLC	C	207	-	-	0/24/24/24	0/0/0/0
7	OLC	C	208	-	-	0/24/24/24	0/0/0/0
7	OLC	C	209	-	-	0/24/24/24	0/0/0/0
7	OLC	C	210	-	-	0/24/24/24	0/0/0/0
7	OLC	C	211	-	-	0/24/24/24	0/0/0/0
2	MLE	D	201	3,6	-	0/4/8/10	0/0/0/0
3	IIL	D	202	2,4	-	0/7/8/10	0/0/0/0
4	SER	D	203	3,5	-	0/2/4/6	0/0/0/0
5	ALO	D	204	4,6	-	0/4/6/8	0/0/0/0
6	5BV	D	205	2,5	-	0/17/18/20	0/0/0/0
7	OLC	D	206	-	-	0/24/24/24	0/0/0/0
7	OLC	D	207	-	-	0/24/24/24	0/0/0/0
7	OLC	D	208	-	-	0/24/24/24	0/0/0/0
7	OLC	D	209	-	-	0/24/24/24	0/0/0/0
7	OLC	D	210	-	-	0/24/24/24	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	204	ALO	CA-C	2.11	1.53	1.50
4	C	203	SER	CA-C	2.45	1.53	1.50
4	D	203	SER	CA-C	2.48	1.53	1.50
4	A	203	SER	CA-C	2.50	1.53	1.50
5	D	204	ALO	CA-C	2.54	1.53	1.50
2	D	201	MLE	CA-C	2.86	1.54	1.50
4	B	203	SER	CA-C	2.87	1.54	1.50
3	D	202	IIL	CA-C	2.89	1.54	1.50
3	A	202	IIL	CA-C	3.03	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	IIL	CA-C	3.13	1.54	1.50
3	C	202	IIL	CA-C	3.15	1.54	1.50
2	A	201	MLE	CA-C	3.15	1.54	1.50
2	C	201	MLE	CA-C	3.21	1.54	1.50
2	B	201	MLE	CA-C	3.22	1.54	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	MLE	O-C-CA	-2.86	118.47	125.15
2	C	201	MLE	O-C-CA	-2.85	118.49	125.15
2	D	201	MLE	O-C-CA	-2.70	118.85	125.15
2	B	201	MLE	O-C-CA	-2.55	119.20	125.15
6	D	205	5BV	O34-C33-C32	2.06	123.72	119.00
6	C	205	5BV	O34-C33-C32	2.20	124.05	119.00
6	A	205	5BV	O34-C33-C32	2.46	124.63	119.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

26 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	MLE	1	0
3	A	202	IIL	1	0
6	A	205	5BV	1	0
7	A	206	OLC	5	0
7	A	207	OLC	3	0
7	A	208	OLC	3	0
7	A	209	OLC	3	0
7	A	210	OLC	2	0
4	B	203	SER	1	0
7	B	206	OLC	2	0
7	B	207	OLC	1	0
7	B	208	OLC	1	0
7	B	209	OLC	2	0
7	B	211	OLC	1	0
7	B	212	OLC	2	0
7	C	206	OLC	1	0
7	C	208	OLC	3	0
7	C	209	OLC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	210	OLC	4	0
7	C	211	OLC	2	0
2	D	201	MLE	1	0
4	D	203	SER	2	0
7	D	206	OLC	2	0
7	D	207	OLC	2	0
7	D	208	OLC	1	0
7	D	210	OLC	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	157/188 (83%)	0.19	3 (1%) 67 58	45, 58, 88, 120	0
1	B	149/188 (79%)	0.28	7 (4%) 32 22	44, 64, 98, 108	0
1	C	149/188 (79%)	0.15	2 (1%) 77 71	44, 58, 96, 128	0
1	D	149/188 (79%)	0.33	10 (6%) 19 11	47, 65, 103, 120	0
All	All	604/752 (80%)	0.24	22 (3%) 43 32	44, 60, 98, 128	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	94	GLY	5.9
1	D	93	LYS	3.9
1	B	58	ALA	3.6
1	D	91	LEU	2.9
1	D	60	SER	2.8
1	C	158	PHE	2.8
1	D	55	THR	2.7
1	B	97	TRP	2.6
1	D	56	GLY	2.6
1	B	91	LEU	2.5
1	A	134	TRP	2.5
1	B	59	PHE	2.5
1	C	92	LYS	2.5
1	D	63	ALA	2.4
1	A	157	MET	2.4
1	B	87	TRP	2.4
1	A	5	ASP	2.3
1	B	57	ALA	2.3
1	D	88	LEU	2.2
1	B	115	ASP	2.1
1	D	68	TRP	2.1
1	D	57	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
7	OLC	C	211	25/25	0.70	0.60	29.11	77,98,120,129	0
7	OLC	D	207	25/25	0.64	0.50	9.02	67,99,110,126	0
7	OLC	C	206	25/25	0.89	0.32	8.33	58,69,86,96	0
7	OLC	C	209	25/25	0.86	0.47	6.63	65,79,105,110	0
7	OLC	A	206	25/25	0.87	0.31	6.24	55,71,86,92	0
7	OLC	A	207	25/25	0.78	0.34	5.84	74,84,100,115	0
7	OLC	D	210	25/25	0.64	0.41	5.54	66,87,112,114	0
7	OLC	B	207	25/25	0.67	0.45	4.95	77,89,127,131	0
7	OLC	B	212	25/25	0.83	0.29	4.69	66,90,103,107	0
7	OLC	D	206	25/25	0.88	0.35	4.50	53,69,94,95	0
7	OLC	A	210	25/25	0.85	0.34	4.34	67,77,88,97	0
7	OLC	C	210	25/25	0.74	0.35	4.24	72,86,101,106	0
7	OLC	B	209	25/25	0.82	0.38	4.04	67,75,105,119	0
7	OLC	A	211	25/25	0.80	0.36	3.98	59,79,95,107	0
7	OLC	A	209	25/25	0.89	0.37	3.71	65,76,89,93	0
7	OLC	B	206	25/25	0.89	0.40	3.23	52,69,118,125	0
7	OLC	D	209	25/25	0.77	0.34	3.14	67,89,114,118	0
7	OLC	B	211	25/25	0.78	0.34	2.69	57,77,115,119	0
7	OLC	B	210	25/25	0.85	0.27	2.50	60,77,85,102	0
7	OLC	C	207	25/25	0.72	0.39	2.26	67,90,109,112	0
5	ALO	C	204	7/8	0.96	0.26	2.03	52,58,66,70	0
2	MLE	C	201	9/10	0.97	0.20	0.90	55,60,63,67	0
2	MLE	B	201	9/10	0.94	0.22	0.86	55,65,70,71	0
2	MLE	A	201	9/10	0.97	0.21	0.77	51,54,58,59	0
6	5BV	D	205	16/17	0.90	0.25	0.08	65,72,101,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	5BV	C	205	16/17	0.97	0.19	-0.42	51,62,77,85	0
4	SER	D	203	6/7	0.94	0.18	-0.50	60,65,70,71	0
3	IIL	D	202	8/9	0.96	0.18	-0.53	55,64,69,71	0
4	SER	A	203	6/7	0.96	0.16	-0.81	49,50,53,59	0
5	ALO	D	204	7/8	0.96	0.19	-0.81	72,76,86,86	0
4	SER	C	203	6/7	0.97	0.19	-0.92	48,50,57,58	0
2	MLE	D	201	9/10	0.95	0.17	-1.19	52,63,68,71	0
6	5BV	A	205	16/17	0.96	0.17	-1.27	50,58,72,77	0
5	ALO	A	204	7/8	0.96	0.16	-1.52	46,49,56,61	0
4	SER	B	203	6/7	0.97	0.14	-1.60	51,52,61,64	0
3	IIL	C	202	8/9	0.96	0.21	-	53,55,60,61	0
3	IIL	B	202	8/9	0.94	0.20	-	53,57,59,63	0
7	OLC	C	208	25/25	0.81	0.34	-	71,95,120,126	0
7	OLC	D	208	25/25	0.77	0.42	-	74,103,134,139	0
6	5BV	B	205	16/17	0.94	0.20	-	61,73,89,93	0
3	IIL	A	202	8/9	0.93	0.22	-	39,48,56,58	0
7	OLC	B	208	25/25	0.75	0.34	-	72,101,119,126	0
5	ALO	B	204	7/8	0.94	0.14	-	60,64,70,70	0
7	OLC	A	208	25/25	0.80	0.37	-	80,99,112,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.