wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:06 PM GMT

PDB ID	:	3VZD
Title	:	Crystal structure of Sphingosine Kinase 1 with inhibitor and ADP
Authors	:	Min, X.; Walker, N.P.; Wang, Z.
Deposited on	:	2012-10-11
Resolution	:	2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

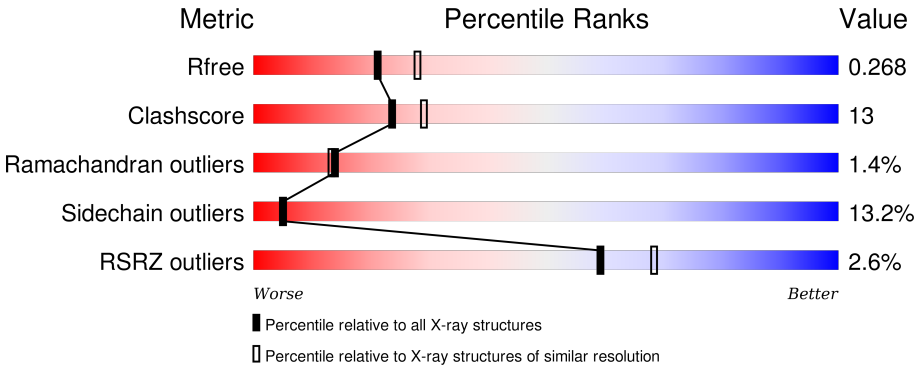
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	361	66% 24% 5% • •
1	B	361	4% 67% 21% 6% • 5%
1	C	361	2% 65% 26% • • •
1	D	361	3% 61% 27% 7% • •
1	E	361	4% 65% 25% 6% 5%

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Mol	Chain	Length	Quality of chain
1	F	361	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16783 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 Sphingosine kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2719	1739	482	477	21			
1	B	342	Total	C	N	O	S	0	0	0
			2675	1714	474	467	20			
1	C	346	Total	C	N	O	S	0	0	0
			2702	1729	479	473	21			
1	D	349	Total	C	N	O	S	0	1	0
			2723	1741	482	479	21			
1	E	344	Total	C	N	O	S	0	0	0
			2691	1724	477	470	20			
1	F	346	Total	C	N	O	S	0	1	0
			2706	1731	479	475	21			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLY	-	EXPRESSION TAG	UNP Q9NYA1
A	5	ALA	-	EXPRESSION TAG	UNP Q9NYA1
A	6	MET	-	EXPRESSION TAG	UNP Q9NYA1
A	7	GLY	-	EXPRESSION TAG	UNP Q9NYA1
A	8	SER	-	EXPRESSION TAG	UNP Q9NYA1
B	4	GLY	-	EXPRESSION TAG	UNP Q9NYA1
B	5	ALA	-	EXPRESSION TAG	UNP Q9NYA1
B	6	MET	-	EXPRESSION TAG	UNP Q9NYA1
B	7	GLY	-	EXPRESSION TAG	UNP Q9NYA1
B	8	SER	-	EXPRESSION TAG	UNP Q9NYA1
C	4	GLY	-	EXPRESSION TAG	UNP Q9NYA1
C	5	ALA	-	EXPRESSION TAG	UNP Q9NYA1
C	6	MET	-	EXPRESSION TAG	UNP Q9NYA1
C	7	GLY	-	EXPRESSION TAG	UNP Q9NYA1
C	8	SER	-	EXPRESSION TAG	UNP Q9NYA1
D	4	GLY	-	EXPRESSION TAG	UNP Q9NYA1
D	5	ALA	-	EXPRESSION TAG	UNP Q9NYA1

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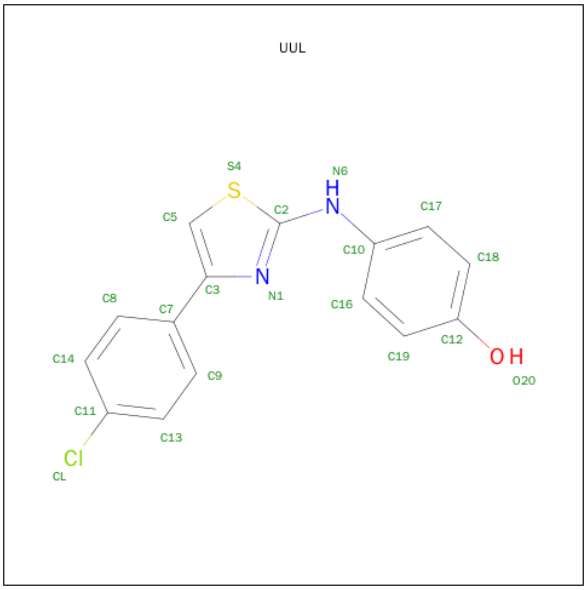
Chain	Residue	Modelled	Actual	Comment	Reference
D	6	MET	-	EXPRESSION TAG	UNP Q9NYA1
D	7	GLY	-	EXPRESSION TAG	UNP Q9NYA1
D	8	SER	-	EXPRESSION TAG	UNP Q9NYA1
E	4	GLY	-	EXPRESSION TAG	UNP Q9NYA1
E	5	ALA	-	EXPRESSION TAG	UNP Q9NYA1
E	6	MET	-	EXPRESSION TAG	UNP Q9NYA1
E	7	GLY	-	EXPRESSION TAG	UNP Q9NYA1
E	8	SER	-	EXPRESSION TAG	UNP Q9NYA1
F	4	GLY	-	EXPRESSION TAG	UNP Q9NYA1
F	5	ALA	-	EXPRESSION TAG	UNP Q9NYA1
F	6	MET	-	EXPRESSION TAG	UNP Q9NYA1
F	7	GLY	-	EXPRESSION TAG	UNP Q9NYA1
F	8	SER	-	EXPRESSION TAG	UNP Q9NYA1

- Molecule 2 is 4-{[4-(4-CHLOROPHENYL)-1,3-THIAZOL-2-YL]AMINO}PHENOL (three-letter code: UUL) (formula: $C_{15}H_{11}ClN_2OS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			20	15	1	2	1	1		
2	A	1	Total	C	Cl	N	O	S	0	0
			20	15	1	2	1	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			20	15	1	2	1	1		
2	C	1	Total	C	Cl	N	O	S	0	0
			20	15	1	2	1	1		

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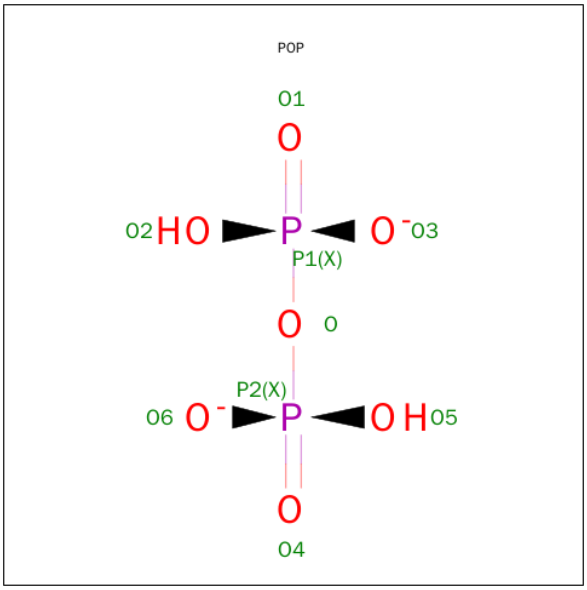
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C Cl N O S 20 15 1 2 1 1	0	0
2	E	1	Total C Cl N O S 20 15 1 2 1 1	0	0
2	F	1	Total C Cl N O S 20 15 1 2 1 1	0	0

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 9 7 2	0	0

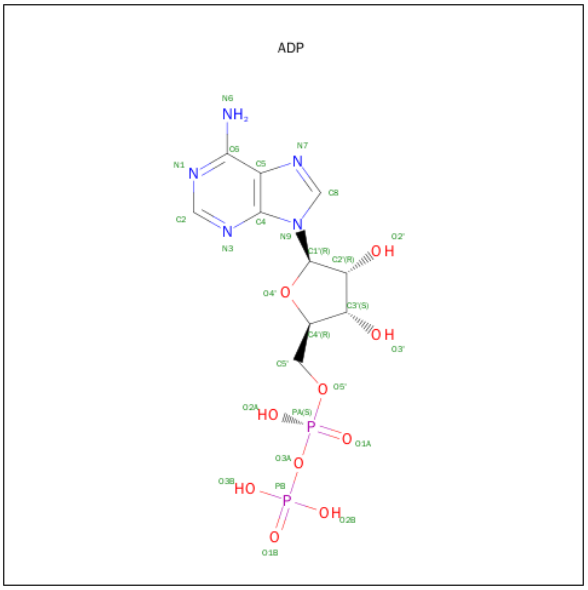
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O P 27 10 5 10 2	0	0
6	E	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	79	Total O 79 79	0	0
7	B	51	Total O 51 51	0	0
7	C	63	Total O 63 63	0	0
7	D	40	Total O 40 40	0	0

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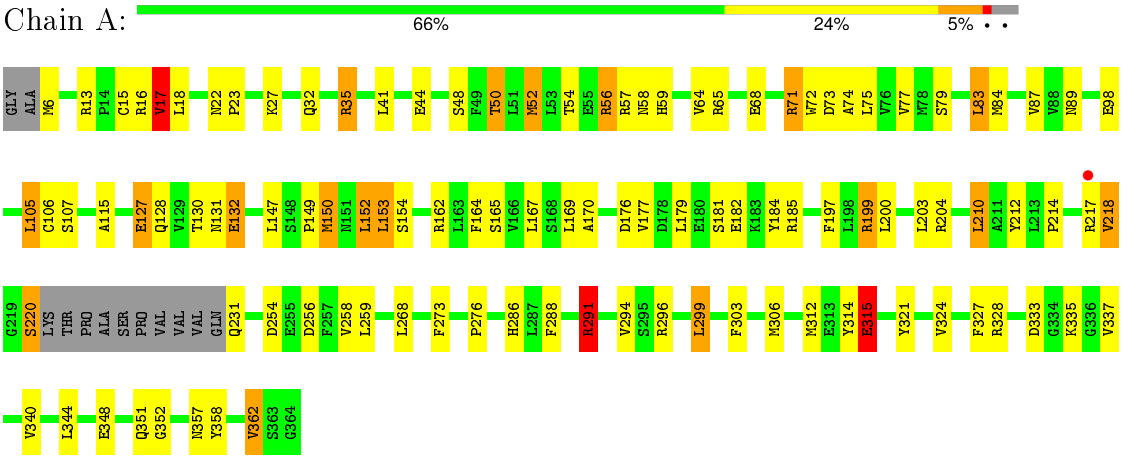
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	75	Total O 75 75	0	0
7	F	50	Total O 50 50	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

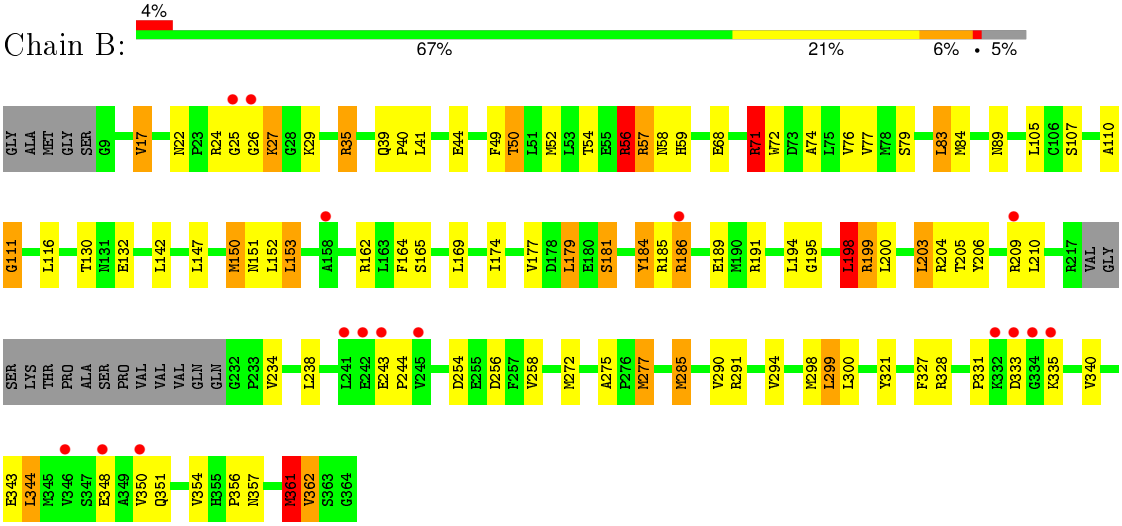
- Molecule 1: Sphingosine kinase 1

Chain A:



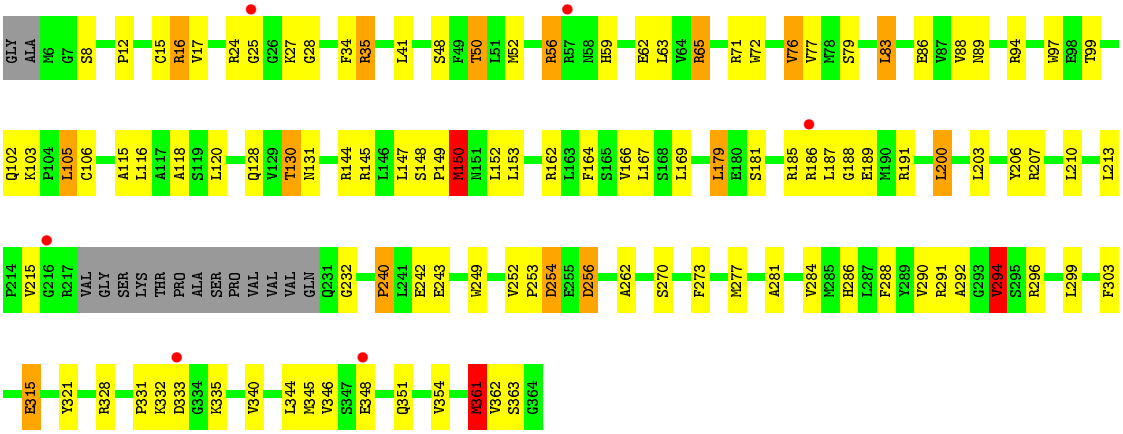
- Molecule 1: Sphingosine kinase 1

Chain B:



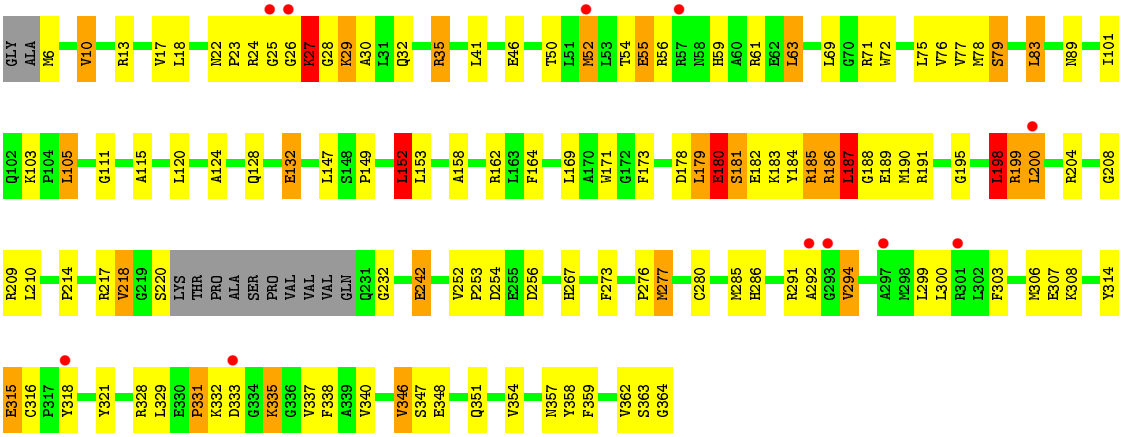
- Molecule 1: Sphingosine kinase 1

Chain C:



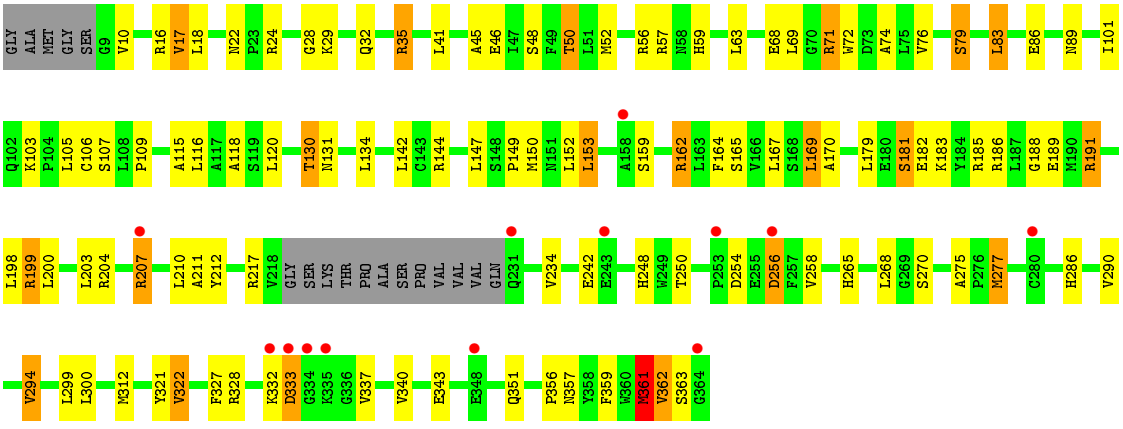
• Molecule 1: Sphingosine kinase 1

Chain D:



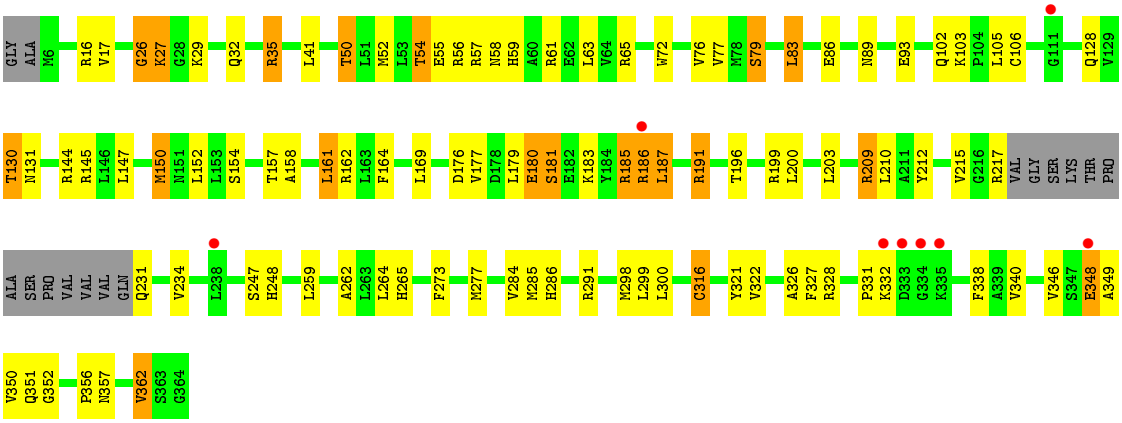
• Molecule 1: Sphingosine kinase 1

Chain E:



• Molecule 1: Sphingosine kinase 1

Chain F:


GLY ALA M6 R16 V17 G26 K27 G28 K29 Q32 R35 L41 T50 L51 M52 L53 T54 E55 R56 R57 N58 H59 A60 R61 E62 L63 V64 R65 W72 V76 V77 W78 S79 L83 E86 N89 E93 Q102 K103 P104 L105 C106 G111 Q128 V129
T130 N131 R144 R145 L146 L147 M150 N151 L152 L153 S154 T157 A158 L161 R162 L163 F164 L169 D176 V177 D178 L179 E180 S181 E182 K183 Y184 R185 R186 L187 R191 T196 R199 L200 L203 R209 L210 A211 Y212 V215 G216 R217 VAL GLY SER LYS THR PRO
ALA SER PRO VAL VAL VAL GLN Q231 V234 L238 S247 H248 L259 A262 L263 L264 H265 F273 M277 V284 M285 H286 R291 M298 L299 L300 C316 Y321 V322 A326 F327 R328 P331 K332 D333 G334 K335 F338 A339 V340 V346 S347 E348 A349
V350 Q351 G352 P356 N357 V362 S363 G364

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.20Å 106.57Å 226.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.30) 98.6 (49.92-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.205 , 0.269 0.205 , 0.268	Depositor DCC
R_{free} test set	5435 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.6	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 108661 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16783	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.32 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.1492e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UUL, MG, POP, ADP, 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	1.00	1/2781 (0.0%)	1.04	11/3770 (0.3%)
1	B	0.93	1/2737 (0.0%)	1.03	9/3712 (0.2%)
1	C	0.99	2/2764 (0.1%)	1.02	13/3747 (0.3%)
1	D	0.95	1/2790 (0.0%)	1.02	8/3782 (0.2%)
1	E	0.95	2/2753 (0.1%)	0.99	6/3734 (0.2%)
1	F	0.94	0/2773	0.98	5/3759 (0.1%)
All	All	0.96	7/16598 (0.0%)	1.01	52/22504 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
1	F	0	2
All	All	0	4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	354	VAL	CB-CG2	-6.25	1.39	1.52
1	E	17	VAL	CB-CG1	-5.72	1.40	1.52
1	D	72	TRP	CE3-CZ3	5.48	1.47	1.38
1	A	324	VAL	CB-CG2	5.28	1.64	1.52
1	C	34	PHE	CE2-CZ	5.21	1.47	1.37

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	35	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	C	35	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	E	361	MET	CG-SD-CE	-8.38	86.80	100.20
1	D	61	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	A	35	ARG	NE-CZ-NH2	-7.84	116.38	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	26	GLY	Peptide
1	D	331	PRO	Peptide
1	F	26	GLY	Peptide
1	F	332	LYS	Peptide

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	2719	0	2749	68	0
1	B	2675	0	2707	85	0
1	C	2702	0	2732	63	0
1	D	2723	0	2751	75	0
1	E	2691	0	2724	86	0
1	F	2706	0	2734	76	0
2	A	40	0	20	3	0
2	B	20	0	11	2	0
2	C	20	0	10	3	0
2	D	20	0	11	0	0
2	E	20	0	11	0	0
2	F	20	0	10	0	0
3	B	9	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	B	1	0	0	1	0
5	C	1	0	0	1	0
5	E	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	27	0	12	1	0
6	E	27	0	12	2	0
7	A	79	0	0	6	0
7	B	51	0	0	1	0
7	C	63	0	0	1	0
7	D	40	0	0	0	0
7	E	75	0	0	1	0
7	F	50	0	0	0	0
All	All	16783	0	16494	435	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.

The worst 5 of 435 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:D:27:LYS:HD2	1:D:27:LYS:H	1.15	1.07
1:E:181:SER:HB3	1:E:191:ARG:HD2	1.33	1.04
1:F:169:LEU:HD12	1:F:340:VAL:HG22	1.40	1.04
1:C:331:PRO:HD2	1:C:348:GLU:O	1.60	1.02
1:A:177:VAL:O	1:A:181:SER:HB2	1.60	1.00

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	345/361 (96%)	332 (96%)	10 (3%)	3 (1%)	21	24
1	B	338/361 (94%)	316 (94%)	19 (6%)	3 (1%)	21	24
1	C	342/361 (95%)	322 (94%)	16 (5%)	4 (1%)	16	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	346/361 (96%)	319 (92%)	15 (4%)	12 (4%)	4 2
1	E	340/361 (94%)	321 (94%)	17 (5%)	2 (1%)	30 36
1	F	343/361 (95%)	320 (93%)	18 (5%)	5 (2%)	13 12
All	All	2054/2166 (95%)	1930 (94%)	95 (5%)	29 (1%)	14 13

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	SER
1	B	111	GLY
1	D	79	SER
1	D	181	SER
1	D	335	LYS

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	290/299 (97%)	252 (87%)	38 (13%)	5 5
1	B	285/299 (95%)	246 (86%)	39 (14%)	4 4
1	C	288/299 (96%)	255 (88%)	33 (12%)	7 7
1	D	291/299 (97%)	249 (86%)	42 (14%)	4 4
1	E	287/299 (96%)	245 (85%)	42 (15%)	4 3
1	F	289/299 (97%)	255 (88%)	34 (12%)	6 7
All	All	1730/1794 (96%)	1502 (87%)	228 (13%)	5 5

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	277	MET
1	D	153	LEU
1	F	185	ARG
1	C	315	GLU

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Mol	Chain	Res	Type
1	D	35	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	351	GLN
1	D	286	HIS
1	F	231	GLN
1	D	59	HIS
1	D	89	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	UUL	A	401	-	19,22,22	1.63	2 (10%)	24,30,30	1.51	4 (16%)
2	UUL	A	402	-	19,22,22	2.23	3 (15%)	24,30,30	2.15	7 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	UUL	B	401	-	19,22,22	1.59	2 (10%)	24,30,30	1.48	5 (20%)
3	POP	B	402	-	8,8,8	0.64	0	13,13,13	1.15	1 (7%)
2	UUL	C	401	-	19,22,22	1.58	2 (10%)	24,30,30	1.63	3 (12%)
6	ADP	C	402	4	22,29,29	1.29	2 (9%)	27,45,45	1.95	6 (22%)
2	UUL	D	500	-	19,22,22	1.55	2 (10%)	24,30,30	1.35	2 (8%)
2	UUL	E	401	-	19,22,22	1.79	2 (10%)	24,30,30	1.39	3 (12%)
6	ADP	E	402	4	22,29,29	1.25	3 (13%)	27,45,45	1.93	5 (18%)
2	UUL	F	500	-	19,22,22	1.86	3 (15%)	24,30,30	1.24	2 (8%)

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	UUL	A	401	-	-	0/6/8/8	0/3/3/3
2	UUL	A	402	-	-	0/6/8/8	0/3/3/3
2	UUL	B	401	-	-	0/6/8/8	0/3/3/3
3	POP	B	402	-	-	0/6/6/6	0/0/0/0
2	UUL	C	401	-	-	0/6/8/8	0/3/3/3
6	ADP	C	402	4	-	0/12/32/32	0/3/3/3
2	UUL	D	500	-	-	0/6/8/8	0/3/3/3
2	UUL	E	401	-	-	0/6/8/8	0/3/3/3
6	ADP	E	402	4	-	0/12/32/32	0/3/3/3
2	UUL	F	500	-	-	0/6/8/8	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	UUL	C7-C3	-7.18	1.38	1.48
2	E	401	UUL	C7-C3	-6.52	1.38	1.48
2	A	401	UUL	C7-C3	-5.97	1.39	1.48
2	F	500	UUL	C7-C3	-5.81	1.40	1.48
2	B	401	UUL	C7-C3	-5.66	1.40	1.48

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	402	ADP	N3-C2-N1	-7.79	122.93	128.89
6	C	402	ADP	N3-C2-N1	-7.63	123.05	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	UUL	C5-C3-C7	-4.83	122.68	129.40
2	A	402	UUL	C8-C7-C3	-4.28	114.26	121.24
2	D	500	UUL	C5-C3-C7	-4.17	123.59	129.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	UUL	2	0
2	A	402	UUL	1	0
2	B	401	UUL	2	0
2	C	401	UUL	3	0
6	C	402	ADP	1	0
6	E	402	ADP	2	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, 95^{th} 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	349/361 (96%)	-0.18	1 (0%) 94 96	18, 32, 52, 66	1 (0%)
1	B	342/361 (94%)	0.35	16 (4%) 35 44	20, 38, 69, 86	1 (0%)
1	C	346/361 (95%)	-0.05	6 (1%) 73 79	20, 35, 57, 66	1 (0%)
1	D	349/361 (96%)	0.07	11 (3%) 51 60	21, 37, 64, 80	1 (0%)
1	E	344/361 (95%)	0.19	13 (3%) 44 53	20, 34, 56, 71	1 (0%)
1	F	346/361 (95%)	0.06	8 (2%) 64 72	22, 39, 63, 80	1 (0%)
All	All	2076/2166 (95%)	0.07	55 (2%) 59 68	18, 36, 62, 86	6 (0%)

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	26	GLY	6.7
1	B	335	LYS	4.7
1	E	334	GLY	4.3
1	D	293	GLY	3.9
1	B	334	GLY	3.8

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	POP	B	402	9/9	0.81	0.29	1.58	157,157,158,158	0
2	UUL	D	500	20/20	0.94	0.17	1.14	37,45,49,49	0
2	UUL	C	401	20/20	0.93	0.15	0.91	32,47,51,51	0
6	ADP	C	402	27/27	0.92	0.20	0.77	47,57,63,65	0
6	ADP	E	402	27/27	0.87	0.19	0.48	58,67,71,71	0
2	UUL	A	402	20/20	0.88	0.15	0.32	49,51,54,63	0
2	UUL	B	401	20/20	0.94	0.16	-0.41	43,57,61,61	0
2	UUL	A	401	20/20	0.97	0.11	-0.53	26,29,33,37	0
5	CL	E	404	1/1	0.94	0.10	-0.69	54,54,54,54	0
2	UUL	E	401	20/20	0.97	0.13	-1.20	26,34,38,39	0
2	UUL	F	500	20/20	0.95	0.10	-1.35	32,44,49,50	0
5	CL	C	404	1/1	0.98	0.07	-1.42	58,58,58,58	0
5	CL	B	404	1/1	0.99	0.08	-1.72	42,42,42,42	0
4	MG	C	403	1/1	0.93	0.16	-	52,52,52,52	0
4	MG	B	403	1/1	0.89	0.19	-	63,63,63,63	0
4	MG	E	403	1/1	0.96	0.18	-	48,48,48,48	0

6.5 Other polymers

There are no such residues in this entry.