



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2026 – 05:56 pm BST

PDB ID : 9S7Y / pdb_00009s7y
Title : Structure of an activated, truncated human 60 kDa lysophospholipase mutant at 2.5 Å resolution
Authors : Rabe von Pappenheim, F.; Tittmann, K.
Deposited on : 2025-08-05
Resolution : 2.50 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

<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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

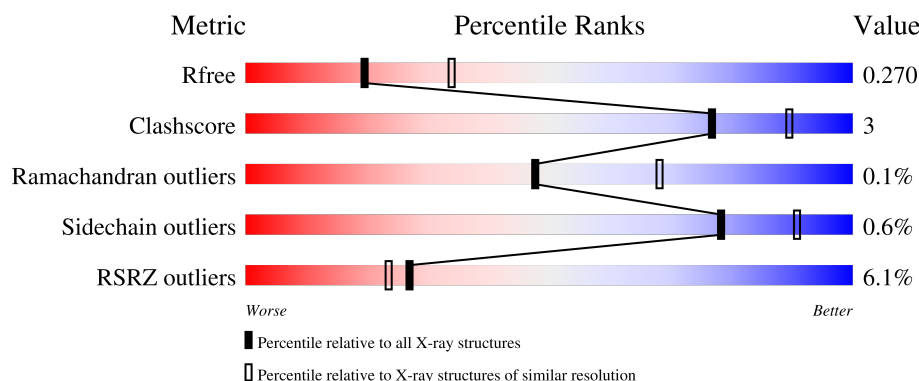
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

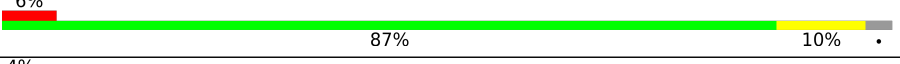
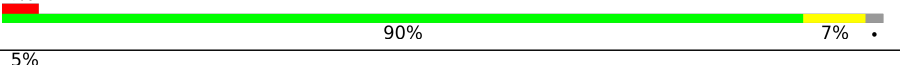
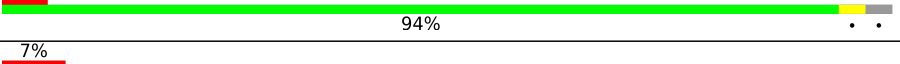
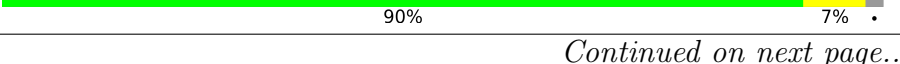
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	366	
1	B	366	
1	C	366	
1	D	366	
1	E	366	

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Mol	Chain	Length	Quality of chain
1	F	366	7% 89% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33234 atoms, of which 16602 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 60 kDa lysophospholipase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	356	Total	C	H	N	O	S	0	0	0
			5488	1722	2778	478	493	17			
1	B	356	Total	C	H	N	O	S	0	0	0
			5488	1722	2778	478	493	17			
1	C	357	Total	C	H	N	O	S	0	0	0
			5500	1726	2782	479	496	17			
1	D	354	Total	C	H	N	O	S	0	0	0
			5442	1711	2750	470	494	17			
1	E	357	Total	C	H	N	O	S	0	0	0
			5500	1726	2782	479	496	17			
1	F	351	Total	C	H	N	O	S	0	0	0
			5394	1696	2726	465	490	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	SER	THR	conflict	UNP Q86U10
A	298	GLN	HIS	conflict	UNP Q86U10
A	301	ARG	GLN	conflict	UNP Q86U10
A	303	SER	ALA	conflict	UNP Q86U10
A	306	PRO	THR	conflict	UNP Q86U10
A	307	GLY	ASP	conflict	UNP Q86U10
A	310	THR	ALA	conflict	UNP Q86U10
A	?	-	GLY	deletion	UNP Q86U10
A	?	-	MET	deletion	UNP Q86U10
A	311	SER	ALA	conflict	UNP Q86U10
A	312	LEU	MET	conflict	UNP Q86U10
A	316	ASN	GLY	conflict	UNP Q86U10
B	297	SER	THR	conflict	UNP Q86U10
B	298	GLN	HIS	conflict	UNP Q86U10
B	301	ARG	GLN	conflict	UNP Q86U10
B	303	SER	ALA	conflict	UNP Q86U10
B	306	PRO	THR	conflict	UNP Q86U10

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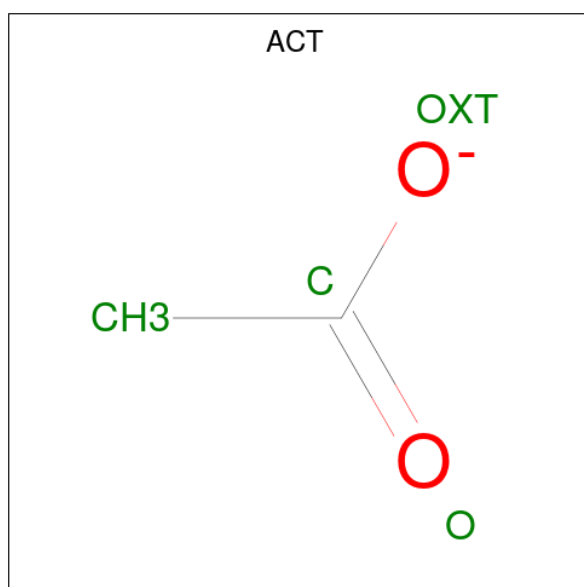
Chain	Residue	Modelled	Actual	Comment	Reference
B	307	GLY	ASP	conflict	UNP Q86U10
B	310	THR	ALA	conflict	UNP Q86U10
B	?	-	GLY	deletion	UNP Q86U10
B	?	-	MET	deletion	UNP Q86U10
B	311	SER	ALA	conflict	UNP Q86U10
B	312	LEU	MET	conflict	UNP Q86U10
B	316	ASN	GLY	conflict	UNP Q86U10
C	297	SER	THR	conflict	UNP Q86U10
C	298	GLN	HIS	conflict	UNP Q86U10
C	301	ARG	GLN	conflict	UNP Q86U10
C	303	SER	ALA	conflict	UNP Q86U10
C	306	PRO	THR	conflict	UNP Q86U10
C	307	GLY	ASP	conflict	UNP Q86U10
C	310	THR	ALA	conflict	UNP Q86U10
C	?	-	GLY	deletion	UNP Q86U10
C	?	-	MET	deletion	UNP Q86U10
C	311	SER	ALA	conflict	UNP Q86U10
C	312	LEU	MET	conflict	UNP Q86U10
C	316	ASN	GLY	conflict	UNP Q86U10
D	297	SER	THR	conflict	UNP Q86U10
D	298	GLN	HIS	conflict	UNP Q86U10
D	301	ARG	GLN	conflict	UNP Q86U10
D	303	SER	ALA	conflict	UNP Q86U10
D	306	PRO	THR	conflict	UNP Q86U10
D	307	GLY	ASP	conflict	UNP Q86U10
D	310	THR	ALA	conflict	UNP Q86U10
D	?	-	GLY	deletion	UNP Q86U10
D	?	-	MET	deletion	UNP Q86U10
D	311	SER	ALA	conflict	UNP Q86U10
D	312	LEU	MET	conflict	UNP Q86U10
D	316	ASN	GLY	conflict	UNP Q86U10
E	297	SER	THR	conflict	UNP Q86U10
E	298	GLN	HIS	conflict	UNP Q86U10
E	301	ARG	GLN	conflict	UNP Q86U10
E	303	SER	ALA	conflict	UNP Q86U10
E	306	PRO	THR	conflict	UNP Q86U10
E	307	GLY	ASP	conflict	UNP Q86U10
E	310	THR	ALA	conflict	UNP Q86U10
E	?	-	GLY	deletion	UNP Q86U10
E	?	-	MET	deletion	UNP Q86U10
E	311	SER	ALA	conflict	UNP Q86U10
E	312	LEU	MET	conflict	UNP Q86U10

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Chain	Residue	Modelled	Actual	Comment	Reference
E	316	ASN	GLY	conflict	UNP Q86U10
F	297	SER	THR	conflict	UNP Q86U10
F	298	GLN	HIS	conflict	UNP Q86U10
F	301	ARG	GLN	conflict	UNP Q86U10
F	303	SER	ALA	conflict	UNP Q86U10
F	306	PRO	THR	conflict	UNP Q86U10
F	307	GLY	ASP	conflict	UNP Q86U10
F	310	THR	ALA	conflict	UNP Q86U10
F	?	-	GLY	deletion	UNP Q86U10
F	?	-	MET	deletion	UNP Q86U10
F	311	SER	ALA	conflict	UNP Q86U10
F	312	LEU	MET	conflict	UNP Q86U10
F	316	ASN	GLY	conflict	UNP Q86U10

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	C	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		

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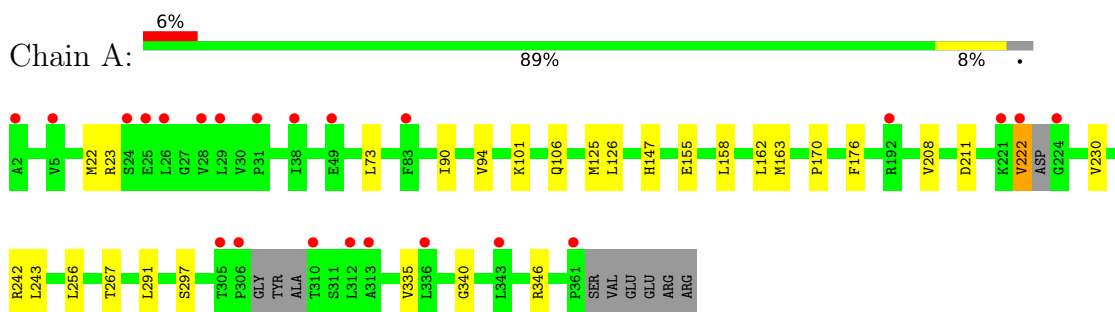
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	54	Total 54	O 54	0	0
3	C	80	Total 80	O 80	0	0
3	D	87	Total 87	O 87	0	0
3	E	53	Total 53	O 53	0	0
3	F	66	Total 66	O 66	0	0

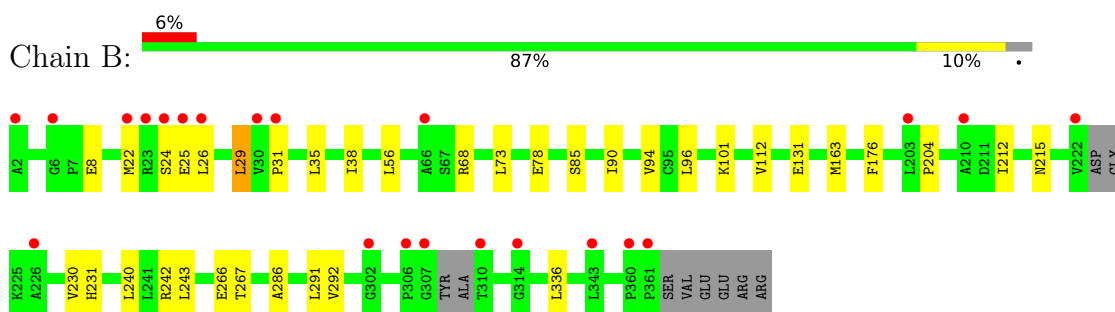
3 Residue-property plots [i](#)

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

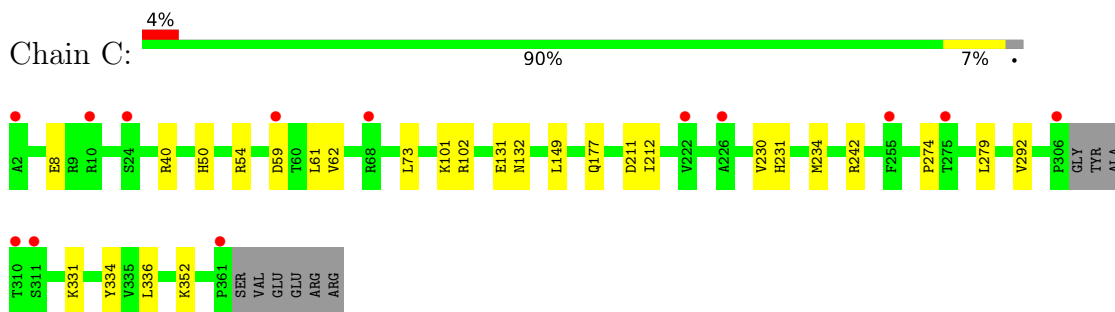
- Molecule 1: 60 kDa lysophospholipase



- Molecule 1: 60 kDa lysophospholipase

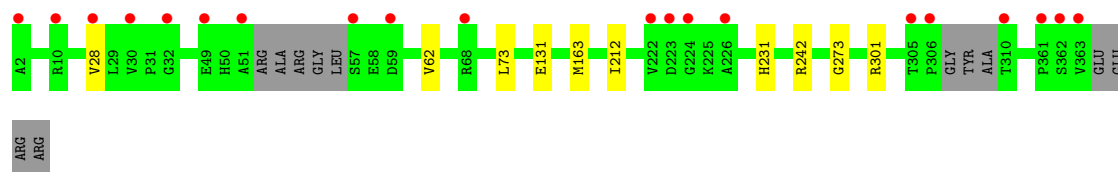


- Molecule 1: 60 kDa lysophospholipase



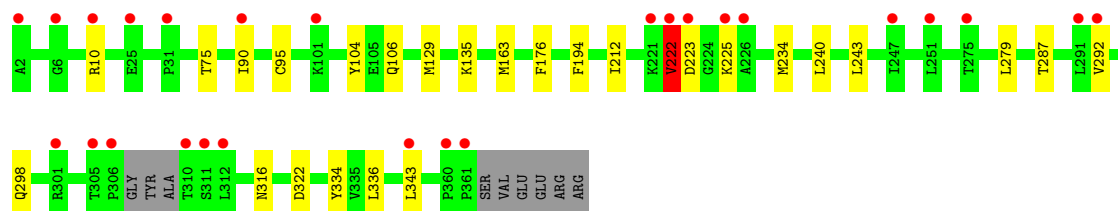
- Molecule 1: 60 kDa lysophospholipase





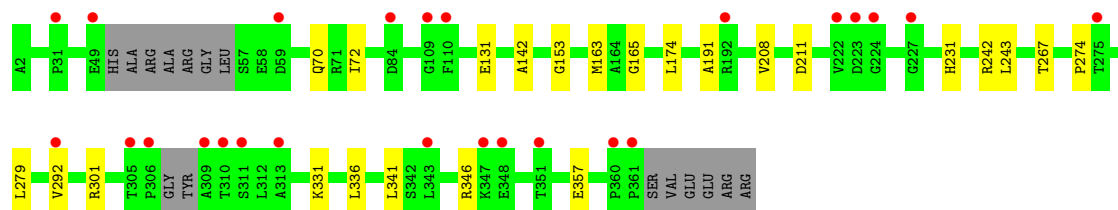
- Molecule 1: 60 kDa lysophospholipase

Chain E: 7% 90% 7%



- Molecule 1: 60 kDa lysophospholipase

Chain F: 7% 89% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	136.91Å 227.90Å 92.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.70 – 2.50 92.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (92.70-2.50) 89.5 (92.70-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.220 , 0.262 0.229 , 0.270	Depositor DCC
R_{free} test set	5154 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.1	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	0.94	EDS
Total number of atoms	33234	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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 35.61 % 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 5.6774e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ACT

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	0.14	0/2758	0.24	0/3741
1	B	0.14	0/2758	0.25	0/3741
1	C	0.15	0/2767	0.26	0/3755
1	D	0.14	0/2740	0.26	0/3719
1	E	0.13	0/2767	0.24	0/3755
1	F	0.15	0/2715	0.25	0/3684
All	All	0.14	0/16505	0.25	0/22395

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	2710	2778	2783	17	0
1	B	2710	2778	2783	20	0
1	C	2718	2782	2788	19	0
1	D	2692	2750	2756	8	0
1	E	2718	2782	2788	20	0
1	F	2668	2726	2731	16	2
2	A	4	3	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	3	3	0	0
3	A	68	0	0	2	1
3	B	54	0	0	4	0
3	C	80	0	0	4	0
3	D	87	0	0	3	1
3	E	53	0	0	7	0
3	F	66	0	0	4	2
All	All	16632	16602	16635	96	3

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 3.

The worst 5 of 96 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:F:301:ARG:O	3:F:401:HOH:O	1.89	0.90
1:D:163:MET:SD	3:D:484:HOH:O	2.30	0.88
1:B:68:ARG:O	3:B:401:HOH:O	1.97	0.83
1:F:331:LYS:NZ	1:F:357:GLU:OE2	2.20	0.74
1:A:162:LEU:HD11	1:C:149:LEU:CD2	2.17	0.74

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:ALA:N	3:F:401:HOH:O[2_665]	2.07	0.13
3:A:520:HOH:O	3:D:409:HOH:O[4_456]	2.14	0.06
1:F:191:ALA:H	3:F:401:HOH:O[2_665]	1.57	0.03

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	350/366 (96%)	341 (97%)	8 (2%)	1 (0%)	36	55
1	B	350/366 (96%)	333 (95%)	16 (5%)	1 (0%)	36	55
1	C	353/366 (96%)	341 (97%)	12 (3%)	0	100	100
1	D	348/366 (95%)	339 (97%)	9 (3%)	0	100	100
1	E	353/366 (96%)	341 (97%)	11 (3%)	1 (0%)	36	55
1	F	345/366 (94%)	335 (97%)	10 (3%)	0	100	100
All	All	2099/2196 (96%)	2030 (97%)	66 (3%)	3 (0%)	48	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	GLU
1	A	340	GLY
1	E	222	VAL

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	292/300 (97%)	287 (98%)	5 (2%)	53	78
1	B	292/300 (97%)	289 (99%)	3 (1%)	68	86
1	C	293/300 (98%)	293 (100%)	0	100	100
1	D	292/300 (97%)	292 (100%)	0	100	100
1	E	293/300 (98%)	290 (99%)	3 (1%)	68	86
1	F	289/300 (96%)	289 (100%)	0	100	100
All	All	1751/1800 (97%)	1740 (99%)	11 (1%)	78	91

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	85	SER
1	E	176	PHE

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Mol	Chain	Res	Type
1	E	225	LYS
1	E	222	VAL
1	A	222	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	98	GLN
1	F	178	ASN
1	F	316	ASN
1	C	272	ASN
1	D	132	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](#)

2 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	ACT	C	401	-	3,3,3	1.27	0	3,3,3	1.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	A	401	-	3,3,3	1.27	0	3,3,3	1.31	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ACT	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	356/366 (97%)	0.46	23 (6%) 25 22	37, 52, 93, 168	0
1	B	356/366 (97%)	0.52	22 (6%) 26 23	44, 56, 93, 149	0
1	C	357/366 (97%)	0.34	13 (3%) 46 41	36, 51, 89, 142	0
1	D	354/366 (96%)	0.49	20 (5%) 30 26	42, 53, 94, 138	0
1	E	357/366 (97%)	0.71	26 (7%) 21 19	39, 61, 100, 169	0
1	F	351/366 (95%)	0.64	25 (7%) 22 19	41, 57, 96, 164	0
All	All	2131/2196 (97%)	0.53	129 (6%) 27 23	36, 55, 94, 169	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	307	GLY	7.7
1	F	309	ALA	6.5
1	D	363	VAL	6.3
1	D	51	ALA	6.3
1	B	26	LEU	6.2

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	ACT	A	401	4/4	0.68	0.21	44,52,54,56	0
2	ACT	C	401	4/4	0.73	0.18	41,43,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.