



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 06:21 PM UTC

PDB ID : 5HC5 / pdb_00005hc5
Title : The structure of esterase Est22 mutant-S188A
Authors : Li, J.; Huang, J.
Deposited on : 2016-01-04
Resolution : 2.43 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
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)
Validation Pipeline (wwPDB-VP)	:	2.49

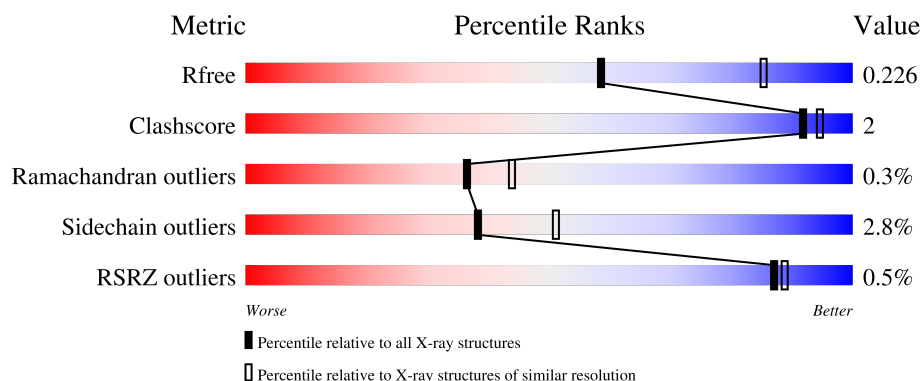
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	365	 87% 6% 7%
1	B	365	 86% 7% 7%
1	C	365	 87% 5% 7%
1	D	365	 86% 7% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10534 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 Lipolytic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	7	0
			2576	1614	434	511	17			
1	B	341	Total	C	N	O	S	0	9	0
			2600	1629	438	516	17			
1	C	338	Total	C	N	O	S	0	9	0
			2580	1617	435	511	17			
1	D	338	Total	C	N	O	S	0	9	0
			2580	1617	435	511	17			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP H6BDX1
A	-19	GLY	-	expression tag	UNP H6BDX1
A	-18	SER	-	expression tag	UNP H6BDX1
A	-17	SER	-	expression tag	UNP H6BDX1
A	-16	HIS	-	expression tag	UNP H6BDX1
A	-15	HIS	-	expression tag	UNP H6BDX1
A	-14	HIS	-	expression tag	UNP H6BDX1
A	-13	HIS	-	expression tag	UNP H6BDX1
A	-12	HIS	-	expression tag	UNP H6BDX1
A	-11	HIS	-	expression tag	UNP H6BDX1
A	-10	HIS	-	expression tag	UNP H6BDX1
A	-9	SER	-	expression tag	UNP H6BDX1
A	-8	SER	-	expression tag	UNP H6BDX1
A	-7	GLY	-	expression tag	UNP H6BDX1
A	-6	LEU	-	expression tag	UNP H6BDX1
A	-5	VAL	-	expression tag	UNP H6BDX1
A	-4	PRO	-	expression tag	UNP H6BDX1
A	-3	ARG	-	expression tag	UNP H6BDX1
A	-2	GLY	-	expression tag	UNP H6BDX1
A	-1	SER	-	expression tag	UNP H6BDX1
A	0	HIS	-	expression tag	UNP H6BDX1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	ALA	SER	engineered mutation	UNP H6BDX1
B	-20	MET	-	expression tag	UNP H6BDX1
B	-19	GLY	-	expression tag	UNP H6BDX1
B	-18	SER	-	expression tag	UNP H6BDX1
B	-17	SER	-	expression tag	UNP H6BDX1
B	-16	HIS	-	expression tag	UNP H6BDX1
B	-15	HIS	-	expression tag	UNP H6BDX1
B	-14	HIS	-	expression tag	UNP H6BDX1
B	-13	HIS	-	expression tag	UNP H6BDX1
B	-12	HIS	-	expression tag	UNP H6BDX1
B	-11	HIS	-	expression tag	UNP H6BDX1
B	-10	HIS	-	expression tag	UNP H6BDX1
B	-9	SER	-	expression tag	UNP H6BDX1
B	-8	SER	-	expression tag	UNP H6BDX1
B	-7	GLY	-	expression tag	UNP H6BDX1
B	-6	LEU	-	expression tag	UNP H6BDX1
B	-5	VAL	-	expression tag	UNP H6BDX1
B	-4	PRO	-	expression tag	UNP H6BDX1
B	-3	ARG	-	expression tag	UNP H6BDX1
B	-2	GLY	-	expression tag	UNP H6BDX1
B	-1	SER	-	expression tag	UNP H6BDX1
B	0	HIS	-	expression tag	UNP H6BDX1
B	188	ALA	SER	engineered mutation	UNP H6BDX1
C	-20	MET	-	expression tag	UNP H6BDX1
C	-19	GLY	-	expression tag	UNP H6BDX1
C	-18	SER	-	expression tag	UNP H6BDX1
C	-17	SER	-	expression tag	UNP H6BDX1
C	-16	HIS	-	expression tag	UNP H6BDX1
C	-15	HIS	-	expression tag	UNP H6BDX1
C	-14	HIS	-	expression tag	UNP H6BDX1
C	-13	HIS	-	expression tag	UNP H6BDX1
C	-12	HIS	-	expression tag	UNP H6BDX1
C	-11	HIS	-	expression tag	UNP H6BDX1
C	-10	HIS	-	expression tag	UNP H6BDX1
C	-9	SER	-	expression tag	UNP H6BDX1
C	-8	SER	-	expression tag	UNP H6BDX1
C	-7	GLY	-	expression tag	UNP H6BDX1
C	-6	LEU	-	expression tag	UNP H6BDX1
C	-5	VAL	-	expression tag	UNP H6BDX1
C	-4	PRO	-	expression tag	UNP H6BDX1
C	-3	ARG	-	expression tag	UNP H6BDX1
C	-2	GLY	-	expression tag	UNP H6BDX1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP H6BDX1
C	0	HIS	-	expression tag	UNP H6BDX1
C	188	ALA	SER	engineered mutation	UNP H6BDX1
D	-20	MET	-	expression tag	UNP H6BDX1
D	-19	GLY	-	expression tag	UNP H6BDX1
D	-18	SER	-	expression tag	UNP H6BDX1
D	-17	SER	-	expression tag	UNP H6BDX1
D	-16	HIS	-	expression tag	UNP H6BDX1
D	-15	HIS	-	expression tag	UNP H6BDX1
D	-14	HIS	-	expression tag	UNP H6BDX1
D	-13	HIS	-	expression tag	UNP H6BDX1
D	-12	HIS	-	expression tag	UNP H6BDX1
D	-11	HIS	-	expression tag	UNP H6BDX1
D	-10	HIS	-	expression tag	UNP H6BDX1
D	-9	SER	-	expression tag	UNP H6BDX1
D	-8	SER	-	expression tag	UNP H6BDX1
D	-7	GLY	-	expression tag	UNP H6BDX1
D	-6	LEU	-	expression tag	UNP H6BDX1
D	-5	VAL	-	expression tag	UNP H6BDX1
D	-4	PRO	-	expression tag	UNP H6BDX1
D	-3	ARG	-	expression tag	UNP H6BDX1
D	-2	GLY	-	expression tag	UNP H6BDX1
D	-1	SER	-	expression tag	UNP H6BDX1
D	0	HIS	-	expression tag	UNP H6BDX1
D	188	ALA	SER	engineered mutation	UNP H6BDX1

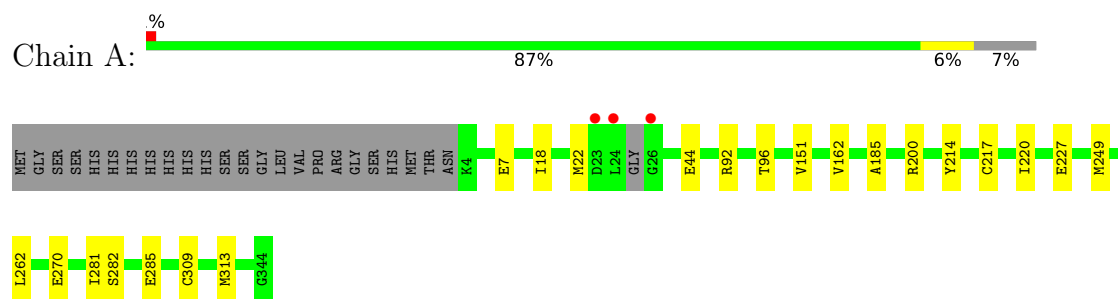
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	52	Total O 52 52	0	0
2	B	50	Total O 50 50	0	0
2	C	47	Total O 47 47	0	0
2	D	49	Total O 49 49	0	0

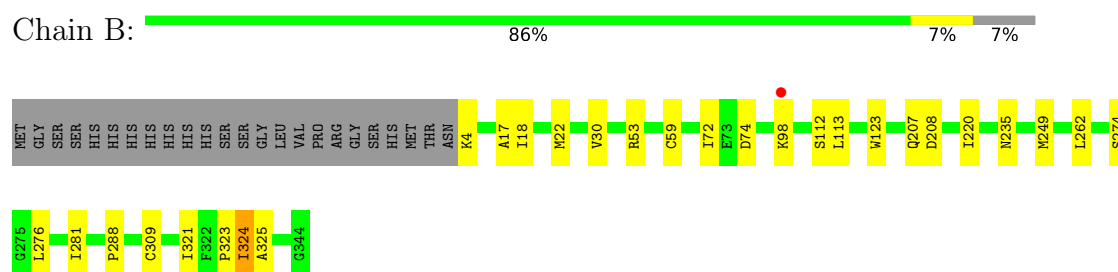
3 Residue-property plots [i](#)

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.

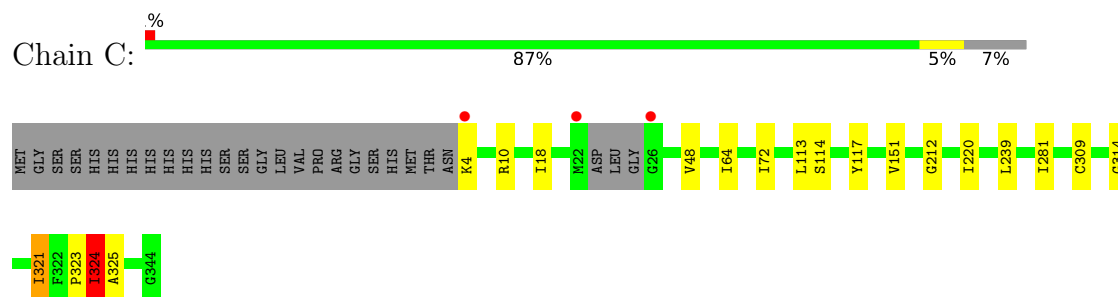
- Molecule 1: Lipolytic enzyme



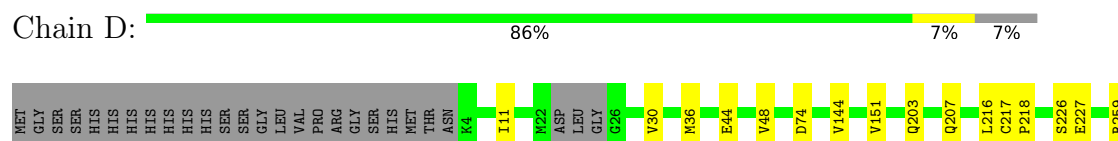
- Molecule 1: Lipolytic enzyme



- Molecule 1: Lipolytic enzyme



- Molecule 1: Lipolytic enzyme





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.47Å 121.80Å 150.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.43 50.00 – 2.43	Depositor EDS
% Data completeness (in resolution range)	87.7 (50.00-2.43) 87.7 (50.00-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.161 , 0.226 0.168 , 0.226	Depositor DCC
R_{free} test set	2476 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10534	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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

5.1 Standard geometry

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	0.81	0/2640	0.99	4/3582 (0.1%)
1	B	0.82	0/2665	0.96	2/3616 (0.1%)
1	C	0.82	0/2644	0.97	4/3586 (0.1%)
1	D	0.81	0/2644	0.94	1/3586 (0.0%)
All	All	0.81	0/10593	0.97	11/14370 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	324	ILE	CB-CA-C	-7.13	102.52	112.14
1	C	324	ILE	N-CA-CB	6.24	119.02	110.54
1	D	11	ILE	N-CA-C	5.97	117.60	108.71
1	C	212	GLY	N-CA-C	5.67	118.88	110.42
1	C	220	ILE	N-CA-C	5.58	119.11	113.47
1	B	324	ILE	CB-CA-C	-5.45	103.71	112.16
1	A	249	MET	N-CA-C	5.39	116.84	111.07
1	B	220	ILE	N-CA-C	5.38	120.53	109.34
1	A	92	ARG	N-CA-C	5.21	114.30	108.25
1	A	18	ILE	N-CA-C	5.20	117.09	111.58
1	A	220	ILE	N-CA-C	5.16	120.08	109.34

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	2576	0	2492	5	0
1	B	2600	0	2523	12	0
1	C	2580	0	2504	11	0
1	D	2580	0	2504	7	0
2	A	52	0	0	0	0
2	B	50	0	0	1	0
2	C	47	0	0	2	0
2	D	49	0	0	1	0
All	All	10534	0	10023	33	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 2.

All (33) 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:72:ILE:HD12	2:B:450:HOH:O	2.00	0.61
1:C:18:ILE:HD12	1:C:325:ALA:HA	1.86	0.58
1:B:123:TRP:CD1	1:B:321:ILE:HG22	2.42	0.54
1:B:207:GLN:OE1	1:B:276[B]:LEU:HD23	2.07	0.54
1:D:281:ILE:O	1:D:309:CYS:HA	2.09	0.52
1:B:17[A]:ALA:HB1	1:C:324:ILE:HD13	1.93	0.51
1:D:259:ARG:HG2	1:D:267:PHE:CE1	2.47	0.49
1:C:64:ILE:CG2	1:C:323:PRO:HB2	2.43	0.49
1:B:17[B]:ALA:HB1	1:C:324:ILE:HD13	1.95	0.48
1:A:162:VAL:HG21	1:A:200:ARG:HG2	1.95	0.47
1:C:4:LYS:N	2:C:401:HOH:O	2.47	0.46
1:A:217:CYS:N	1:A:282:SER:O	2.49	0.46
1:B:59:CYS:HB3	1:B:323:PRO:HD2	1.97	0.45
1:B:281:ILE:O	1:B:309:CYS:HA	2.15	0.45
1:D:216:LEU:O	1:D:217:CYS:C	2.59	0.45
1:D:207:GLN:OE1	1:D:276[A]:LEU:HD12	2.18	0.44
1:A:185:ALA:HA	1:A:214:TYR:O	2.17	0.44
1:B:30:VAL:HG23	1:B:249:MET:HG3	1.98	0.43
1:B:235:ASN:HB2	1:B:288:PRO:HA	1.99	0.43
1:B:98[A]:LYS:HE2	1:B:98[A]:LYS:HB3	1.85	0.43
1:D:30:VAL:HG21	1:D:36:MET:SD	2.58	0.43
1:D:321:ILE:C	1:D:323:PRO:HD3	2.42	0.43
1:C:18:ILE:HD13	1:C:324:ILE:HD12	2.01	0.42
1:A:281:ILE:O	1:A:309:CYS:HA	2.20	0.42
1:D:218:PRO:HD2	2:D:413:HOH:O	2.20	0.42
1:B:18:ILE:CD1	1:B:325:ALA:HA	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ILE:C	1:C:323:PRO:HD3	2.45	0.41
1:C:281:ILE:O	1:C:309:CYS:HA	2.21	0.41
1:C:114:SER:HB3	1:C:117:TYR:CE1	2.55	0.41
1:A:285:GLU:HB2	1:A:313:MET:HA	2.02	0.41
1:C:72:ILE:HG13	2:C:446:HOH:O	2.20	0.41
1:B:321:ILE:C	1:B:321:ILE:HD12	2.46	0.41
1:C:10:ARG:O	1:C:314:GLY:HA2	2.22	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	343/365 (94%)	323 (94%)	20 (6%)	0	100	100
1	B	348/365 (95%)	331 (95%)	16 (5%)	1 (0%)	36	44
1	C	343/365 (94%)	329 (96%)	12 (4%)	2 (1%)	21	25
1	D	343/365 (94%)	324 (94%)	18 (5%)	1 (0%)	36	44
All	All	1377/1460 (94%)	1307 (95%)	66 (5%)	4 (0%)	36	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	239	LEU
1	B	113	LEU
1	C	113	LEU
1	D	343	GLY

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	271/287 (94%)	263 (97%)	8 (3%)	36	48
1	B	274/287 (96%)	265 (97%)	9 (3%)	33	45
1	C	272/287 (95%)	268 (98%)	4 (2%)	57	69
1	D	272/287 (95%)	263 (97%)	9 (3%)	33	45
All	All	1089/1148 (95%)	1059 (97%)	30 (3%)	38	51

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	22	MET
1	A	44	GLU
1	A	96	THR
1	A	151	VAL
1	A	227	GLU
1	A	262	LEU
1	A	270	GLU
1	B	4	LYS
1	B	22	MET
1	B	53	ARG
1	B	74	ASP
1	B	112	SER
1	B	208	ASP
1	B	262	LEU
1	B	274	SER
1	B	324	ILE
1	C	48	VAL
1	C	151	VAL
1	C	321	ILE
1	C	324	ILE
1	D	44	GLU
1	D	48	VAL
1	D	74	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	144	VAL
1	D	151	VAL
1	D	203	GLN
1	D	226	SER
1	D	227	GLU
1	D	271	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	119	ASN
1	D	246	GLN

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](#)

There are no ligands in this entry.

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	340/365 (93%)	-0.58	3 (0%) 81 82	15, 37, 60, 98	7 (2%)
1	B	341/365 (93%)	-0.66	1 (0%) 90 91	15, 34, 59, 100	9 (2%)
1	C	338/365 (92%)	-0.59	3 (0%) 81 82	16, 37, 61, 88	9 (2%)
1	D	338/365 (92%)	-0.59	0 100 100	17, 37, 60, 83	9 (2%)
All	All	1357/1460 (92%)	-0.60	7 (0%) 87 89	15, 36, 61, 100	34 (2%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98[A]	LYS	12.0
1	A	26	GLY	3.5
1	A	23	ASP	2.6
1	C	26	GLY	2.6
1	C	4	LYS	2.4
1	C	22	MET	2.4
1	A	24	LEU	2.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.