Full wwPDB X-ray Structure Validation Report (i)

Feb 9, 2017 – 12:06 PM EST

PDB ID	:	5FV4
Title	:	Pig liver esterase 5 (PLE5)
Authors	:	Werten, S.; Palm, G.J.; Berndt, L.; Hinrichs, W.
Deposited on	:	2016-02-03
Resolution	:	2.40 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 (i) symbol.

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

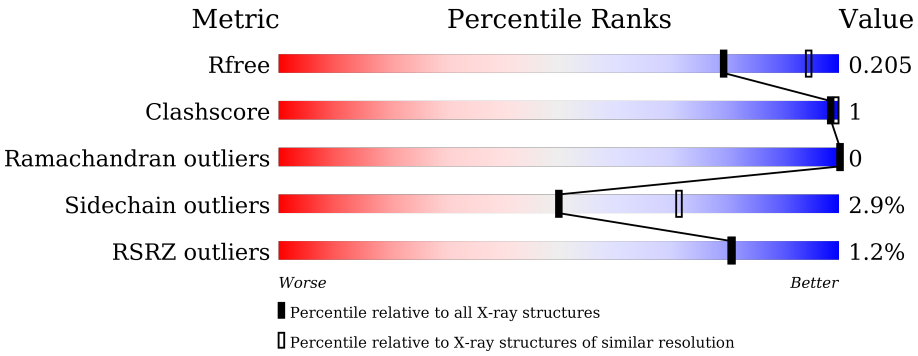
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	544	92% 5%
1	B	544	93%
1	C	544	92% 5%
1	D	544	91% 6%
1	E	544	3% 92% 5%
1	F	544	93%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25087 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 CARBOXYLIC ESTER HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4095	2636	682	760	17			
1	B	530	Total	C	N	O	S	0	0	0
			4095	2636	682	760	17			
1	C	530	Total	C	N	O	S	0	0	0
			4095	2636	682	760	17			
1	D	530	Total	C	N	O	S	0	0	0
			4095	2636	682	760	17			
1	E	530	Total	C	N	O	S	0	0	0
			4095	2636	682	760	17			
1	F	530	Total	C	N	O	S	0	0	0
			4095	2636	682	760	17			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	ASP	GLU	CONFLICT	UNP A9GYW6
A	75	VAL	ILE	CONFLICT	UNP A9GYW6
A	76	ALA	GLY	CONFLICT	UNP A9GYW6
A	80	THR	LEU	CONFLICT	UNP A9GYW6
A	459	ALA	PHE	CONFLICT	UNP A9GYW6
A	461	PHE	LEU	CONFLICT	UNP A9GYW6
A	463	ARG	LYS	CONFLICT	UNP A9GYW6
B	73	ASP	GLU	CONFLICT	UNP A9GYW6
B	75	VAL	ILE	CONFLICT	UNP A9GYW6
B	76	ALA	GLY	CONFLICT	UNP A9GYW6
B	80	THR	LEU	CONFLICT	UNP A9GYW6
B	459	ALA	PHE	CONFLICT	UNP A9GYW6
B	461	PHE	LEU	CONFLICT	UNP A9GYW6
B	463	ARG	LYS	CONFLICT	UNP A9GYW6
C	73	ASP	GLU	CONFLICT	UNP A9GYW6
C	75	VAL	ILE	CONFLICT	UNP A9GYW6
C	76	ALA	GLY	CONFLICT	UNP A9GYW6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	80	THR	LEU	CONFLICT	UNP A9GYW6
C	459	ALA	PHE	CONFLICT	UNP A9GYW6
C	461	PHE	LEU	CONFLICT	UNP A9GYW6
C	463	ARG	LYS	CONFLICT	UNP A9GYW6
D	73	ASP	GLU	CONFLICT	UNP A9GYW6
D	75	VAL	ILE	CONFLICT	UNP A9GYW6
D	76	ALA	GLY	CONFLICT	UNP A9GYW6
D	80	THR	LEU	CONFLICT	UNP A9GYW6
D	459	ALA	PHE	CONFLICT	UNP A9GYW6
D	461	PHE	LEU	CONFLICT	UNP A9GYW6
D	463	ARG	LYS	CONFLICT	UNP A9GYW6
E	73	ASP	GLU	CONFLICT	UNP A9GYW6
E	75	VAL	ILE	CONFLICT	UNP A9GYW6
E	76	ALA	GLY	CONFLICT	UNP A9GYW6
E	80	THR	LEU	CONFLICT	UNP A9GYW6
E	459	ALA	PHE	CONFLICT	UNP A9GYW6
E	461	PHE	LEU	CONFLICT	UNP A9GYW6
E	463	ARG	LYS	CONFLICT	UNP A9GYW6
F	73	ASP	GLU	CONFLICT	UNP A9GYW6
F	75	VAL	ILE	CONFLICT	UNP A9GYW6
F	76	ALA	GLY	CONFLICT	UNP A9GYW6
F	80	THR	LEU	CONFLICT	UNP A9GYW6
F	459	ALA	PHE	CONFLICT	UNP A9GYW6
F	461	PHE	LEU	CONFLICT	UNP A9GYW6
F	463	ARG	LYS	CONFLICT	UNP A9GYW6

- Molecule 2 is water.

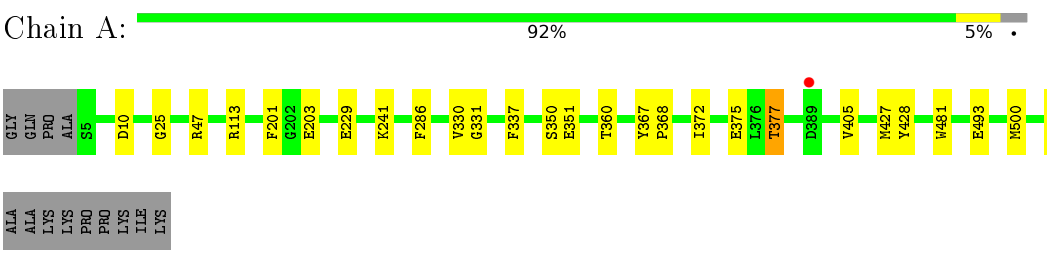
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	92	Total O 92 92	0	0
2	B	103	Total O 103 103	0	0
2	C	124	Total O 124 124	0	0
2	D	34	Total O 34 34	0	0
2	E	54	Total O 54 54	0	0
2	F	110	Total O 110 110	0	0

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.

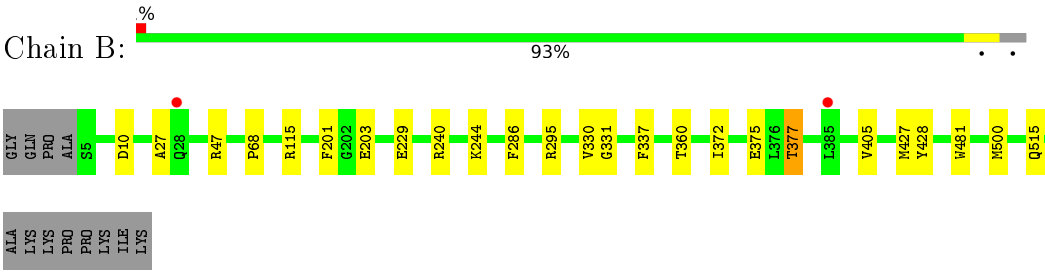
- Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain A:



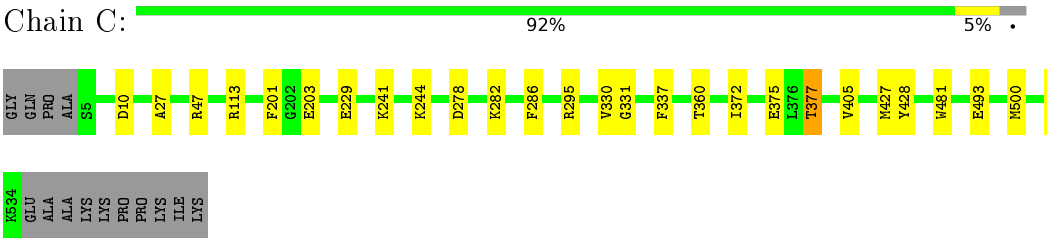
- Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain B:



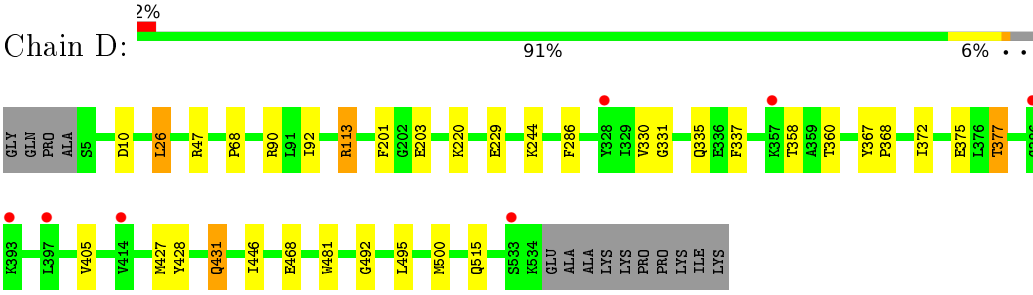
- Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain C:



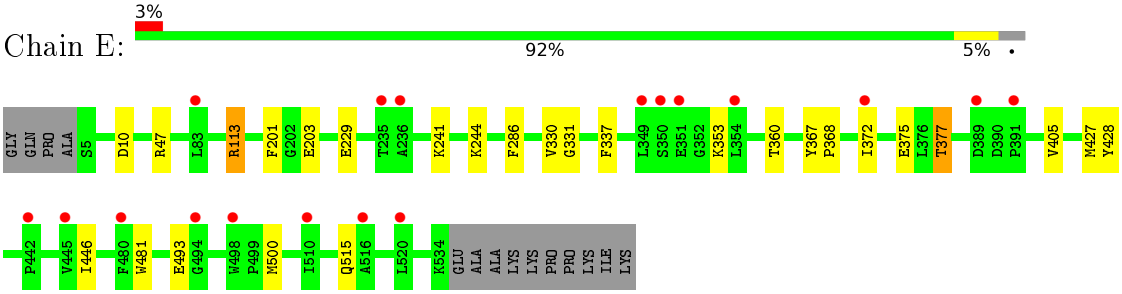
- Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain D:



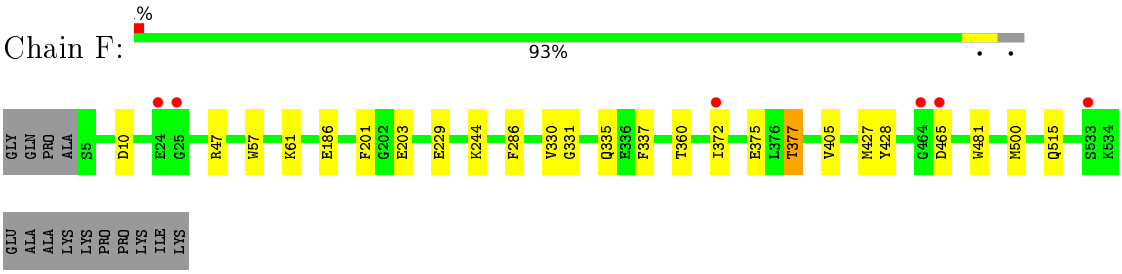
• Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain E:



• Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.86Å 188.02Å 109.50Å 90.00° 96.44° 90.00°	Depositor
Resolution (Å)	71.14 – 2.40 71.14 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (71.14-2.40) 99.7 (71.14-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.179 , 0.205 0.181 , 0.205	Depositor DCC
R_{free} test set	7248 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 30.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25087	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.75	0/4207	0.77	1/5724 (0.0%)
1	B	0.70	0/4207	0.78	5/5724 (0.1%)
1	C	0.67	0/4207	0.77	3/5724 (0.1%)
1	D	0.66	0/4207	0.78	3/5724 (0.1%)
1	E	0.61	0/4207	0.74	2/5724 (0.0%)
1	F	0.69	0/4207	0.78	4/5724 (0.1%)
All	All	0.68	0/25242	0.77	18/34344 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	465	ASP	CB-CG-OD2	9.25	126.62	118.30
1	D	26	LEU	CB-CG-CD1	8.28	125.08	111.00
1	C	295	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	47	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	B	295	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	F	465	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	E	113	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	47	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	D	113	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	F	47	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	47	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	E	47	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	295	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	47	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	F	47	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	D	47	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	240	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	47	ARG	NE-CZ-NH1	5.17	122.89	120.30

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	4095	0	4041	12	0
1	B	4095	0	4041	6	0
1	C	4095	0	4041	10	0
1	D	4095	0	4041	15	2
1	E	4095	0	4041	8	2
1	F	4095	0	4041	6	0
2	A	92	0	0	0	0
2	B	103	0	0	0	0
2	C	124	0	0	0	0
2	D	34	0	0	0	0
2	E	54	0	0	0	0
2	F	110	0	0	0	0
All	All	25087	0	24246	46	2

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 1.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:SER:C	1:D:90:ARG:HH12	1.96	0.69
1:A:350:SER:O	1:D:90:ARG:NH1	2.33	0.62
1:A:360:THR:HG23	1:A:377:THR:HG23	1.93	0.51
1:A:351:GLU:HG2	1:D:92:ILE:HD11	1.92	0.51
1:B:360:THR:HG23	1:B:377:THR:HG23	1.93	0.50
1:D:360:THR:HG23	1:D:377:THR:HG23	1.94	0.50
1:C:360:THR:HG23	1:C:377:THR:HG23	1.93	0.50
1:E:360:THR:HG23	1:E:377:THR:HG23	1.94	0.50
1:F:331:GLY:HA3	1:F:428:TYR:CE2	2.47	0.49
1:A:25:GLY:HA2	1:E:446:ILE:HD13	1.95	0.49
1:C:493:GLU:HB3	1:D:468:GLU:HG2	1.95	0.49
1:C:27:ALA:CB	1:D:431:GLN:OE1	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLU:HA	1:D:90:ARG:HH11	1.79	0.48
1:F:360:THR:HG23	1:F:377:THR:HG23	1.94	0.48
1:B:331:GLY:HA3	1:B:428:TYR:CE2	2.50	0.47
1:A:331:GLY:HA3	1:A:428:TYR:CE2	2.51	0.46
1:B:372:ILE:HD11	1:B:405:VAL:HG21	1.98	0.45
1:C:372:ILE:HD11	1:C:405:VAL:HG21	1.98	0.45
1:B:330:VAL:O	1:B:427:MET:HA	2.17	0.44
1:C:203:GLU:HA	1:C:229:GLU:O	2.17	0.44
1:F:203:GLU:HA	1:F:229:GLU:O	2.18	0.44
1:F:372:ILE:HD11	1:F:405:VAL:HG21	1.99	0.44
1:D:330:VAL:O	1:D:427:MET:HA	2.18	0.44
1:D:331:GLY:HA3	1:D:428:TYR:CE2	2.52	0.44
1:A:203:GLU:HA	1:A:229:GLU:O	2.17	0.43
1:E:330:VAL:O	1:E:427:MET:HA	2.18	0.43
1:A:330:VAL:O	1:A:427:MET:HA	2.17	0.43
1:E:203:GLU:HA	1:E:229:GLU:O	2.18	0.43
1:C:331:GLY:HA3	1:C:428:TYR:CE2	2.54	0.43
1:E:331:GLY:HA3	1:E:428:TYR:CE2	2.53	0.43
1:F:330:VAL:O	1:F:427:MET:HA	2.19	0.43
1:D:367:TYR:N	1:D:368:PRO:HD2	2.35	0.42
1:D:203:GLU:HA	1:D:229:GLU:O	2.18	0.42
1:D:372:ILE:HD11	1:D:405:VAL:HG21	2.00	0.42
1:E:372:ILE:HD11	1:E:405:VAL:HG21	2.01	0.42
1:A:372:ILE:HD11	1:A:405:VAL:HG21	2.00	0.42
1:B:203:GLU:HA	1:B:229:GLU:O	2.19	0.42
1:C:330:VAL:O	1:C:427:MET:HA	2.19	0.42
1:B:27:ALA:HB1	1:C:517:ALA:HB2	2.01	0.42
1:C:27:ALA:HB1	1:D:431:GLN:OE1	2.20	0.42
1:F:57:TRP:CD2	1:F:61:LYS:HE2	2.54	0.42
1:D:358:THR:OG1	1:E:353:LYS:NZ	2.48	0.41
1:E:367:TYR:N	1:E:368:PRO:HD2	2.36	0.41
1:C:278:ASP:OD2	1:C:282:LYS:CE	2.69	0.40
1:A:350:SER:C	1:D:90:ARG:NH1	2.69	0.40
1:A:367:TYR:N	1:A:368:PRO:HD2	2.36	0.40

All (2) 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:D:492:GLY:O	1:E:493:GLU:OE1[1_455]	1.85	0.35
1:D:495:LEU:O	1:E:493:GLU:OE2[1_455]	1.91	0.29

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	528/544 (97%)	509 (96%)	19 (4%)	0	100	100
1	B	528/544 (97%)	509 (96%)	19 (4%)	0	100	100
1	C	528/544 (97%)	509 (96%)	19 (4%)	0	100	100
1	D	528/544 (97%)	508 (96%)	20 (4%)	0	100	100
1	E	528/544 (97%)	509 (96%)	19 (4%)	0	100	100
1	F	528/544 (97%)	509 (96%)	19 (4%)	0	100	100
All	All	3168/3264 (97%)	3053 (96%)	115 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	440/450 (98%)	428 (97%)	12 (3%)	52	73
1	B	440/450 (98%)	428 (97%)	12 (3%)	52	73
1	C	440/450 (98%)	428 (97%)	12 (3%)	52	73
1	D	440/450 (98%)	423 (96%)	17 (4%)	39	59
1	E	440/450 (98%)	428 (97%)	12 (3%)	52	73
1	F	440/450 (98%)	428 (97%)	12 (3%)	52	73
All	All	2640/2700 (98%)	2563 (97%)	77 (3%)	50	71

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	113	ARG
1	A	201	PHE
1	A	241	LYS
1	A	286	PHE
1	A	337	PHE
1	A	375	GLU
1	A	377	THR
1	A	481	TRP
1	A	493	GLU
1	A	500	MET
1	A	515	GLN
1	B	10	ASP
1	B	68	PRO
1	B	115	ARG
1	B	201	PHE
1	B	244	LYS
1	B	286	PHE
1	B	337	PHE
1	B	375	GLU
1	B	377	THR
1	B	481	TRP
1	B	500	MET
1	B	515	GLN
1	C	10	ASP
1	C	113	ARG
1	C	201	PHE
1	C	241	LYS
1	C	244	LYS
1	C	286	PHE
1	C	337	PHE
1	C	375	GLU
1	C	377	THR
1	C	481	TRP
1	C	500	MET
1	C	515	GLN
1	D	10	ASP
1	D	26	LEU
1	D	68	PRO
1	D	113	ARG
1	D	201	PHE
1	D	220	LYS

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Mol	Chain	Res	Type
1	D	244	LYS
1	D	286	PHE
1	D	335	GLN
1	D	337	PHE
1	D	375	GLU
1	D	377	THR
1	D	431	GLN
1	D	446	ILE
1	D	481	TRP
1	D	500	MET
1	D	515	GLN
1	E	10	ASP
1	E	113	ARG
1	E	201	PHE
1	E	241	LYS
1	E	244	LYS
1	E	286	PHE
1	E	337	PHE
1	E	375	GLU
1	E	377	THR
1	E	481	TRP
1	E	500	MET
1	E	515	GLN
1	F	10	ASP
1	F	186	GLU
1	F	201	PHE
1	F	244	LYS
1	F	286	PHE
1	F	335	GLN
1	F	337	PHE
1	F	375	GLU
1	F	377	THR
1	F	481	TRP
1	F	500	MET
1	F	515	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	530/544 (97%)	-0.48	1 (0%) 95 95	36, 52, 87, 133	0
1	B	530/544 (97%)	-0.39	3 (0%) 90 90	38, 59, 99, 154	0
1	C	530/544 (97%)	-0.44	0 100 100	36, 57, 95, 141	0
1	D	530/544 (97%)	-0.20	9 (1%) 73 72	38, 70, 127, 159	0
1	E	530/544 (97%)	-0.03	18 (3%) 49 49	43, 80, 127, 151	0
1	F	530/544 (97%)	-0.41	6 (1%) 82 82	38, 58, 113, 142	0
All	All	3180/3264 (97%)	-0.33	37 (1%) 81 81	36, 61, 116, 159	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	494	GLY	5.7
1	E	498	TRP	4.8
1	E	391	PRO	4.5
1	E	389	ASP	4.5
1	F	24	GLU	4.5
1	D	387	GLY	4.5
1	D	389	ASP	4.0
1	E	354	LEU	3.9
1	E	442	PRO	3.6
1	B	534	LYS	3.4
1	E	350	SER	3.3
1	E	372	ILE	3.2
1	F	465	ASP	3.2
1	B	28	GLN	3.2
1	E	480	PHE	3.1
1	E	520	LEU	2.9
1	D	397	LEU	2.9
1	D	357	LYS	2.9
1	F	464	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	349	LEU	2.7
1	F	25	GLY	2.7
1	D	328	TYR	2.6
1	D	393	LYS	2.5
1	E	236	ALA	2.5
1	E	445	VAL	2.4
1	E	510	ILE	2.4
1	D	414	VAL	2.3
1	E	351	GLU	2.3
1	E	83	LEU	2.3
1	B	385	LEU	2.2
1	D	386	GLY	2.2
1	D	533	SER	2.2
1	E	235	THR	2.1
1	F	372	ILE	2.1
1	F	533	SER	2.1
1	E	516	ALA	2.1
1	A	389	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates 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.