



Full wwPDB X-ray Structure Validation Report i

Sep 20, 2023 – 05:07 PM EDT

PDB ID : 5KJD
Title : Synechocystis apocarotenoid oxygenase (ACO) mutant - Glu150Gln
Authors : Sui, X.; Kiser, P.D.; Palczewski, K.
Deposited on : 2016-06-18
Resolution : 2.75 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 i 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

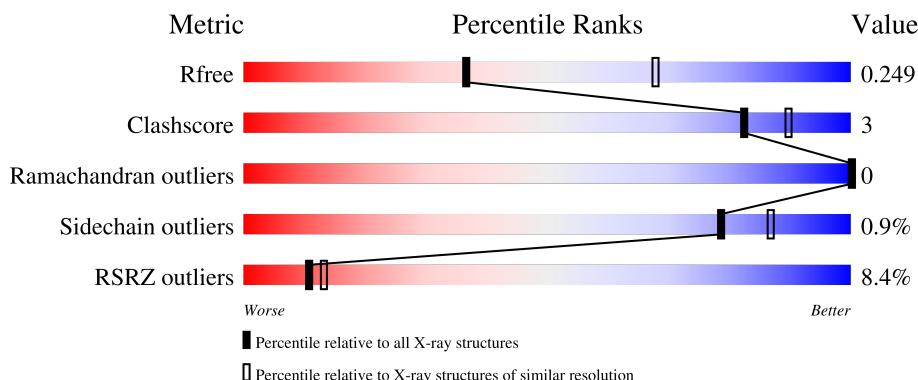
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

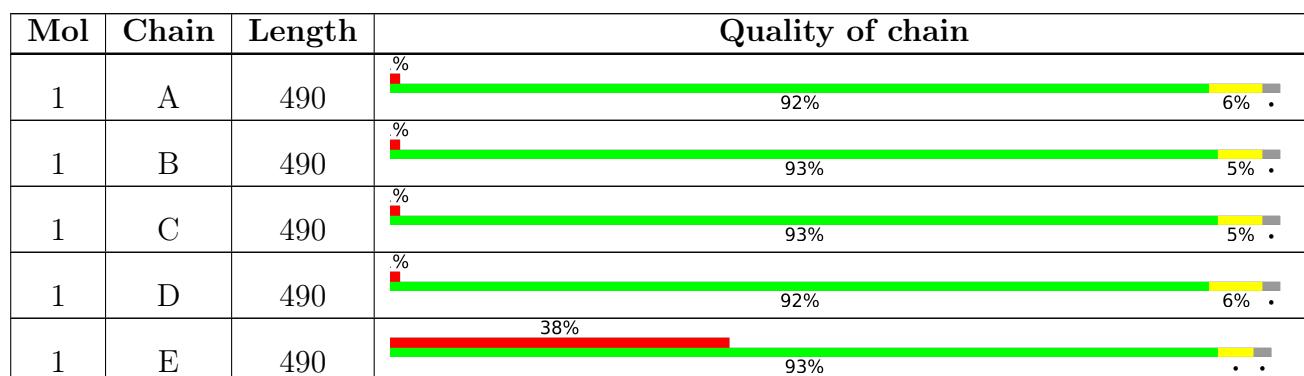
The reported resolution of this entry is 2.75 Å.

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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 <=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.



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18952 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 Apocarotenoid-15,15'-oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3768	2417	651	690	10			
1	B	479	Total	C	N	O	S	0	0	0
			3768	2417	651	690	10			
1	C	479	Total	C	N	O	S	0	0	0
			3768	2417	651	690	10			
1	D	479	Total	C	N	O	S	0	0	0
			3768	2417	651	690	10			
1	E	479	Total	C	N	O	S	0	0	0
			3768	2417	651	690	10			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	GLN	GLU	engineered mutation	UNP P74334
B	150	GLN	GLU	engineered mutation	UNP P74334
C	150	GLN	GLU	engineered mutation	UNP P74334
D	150	GLN	GLU	engineered mutation	UNP P74334
E	150	GLN	GLU	engineered mutation	UNP P74334

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0

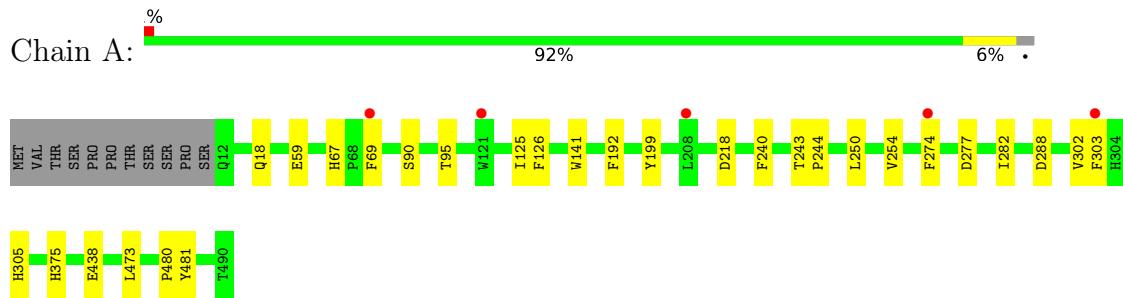
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	33	Total O 33 33	0	0
3	B	29	Total O 29 29	0	0
3	C	25	Total O 25 25	0	0
3	D	18	Total O 18 18	0	0
3	E	2	Total O 2 2	0	0

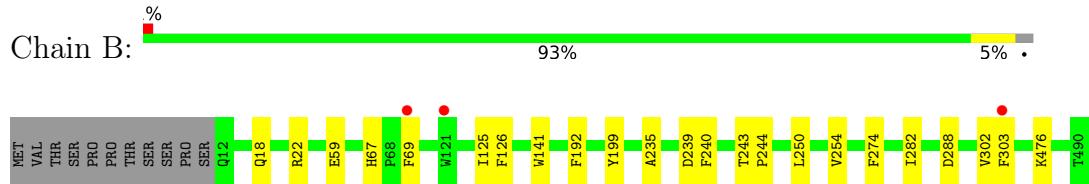
3 Residue-property plots

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.

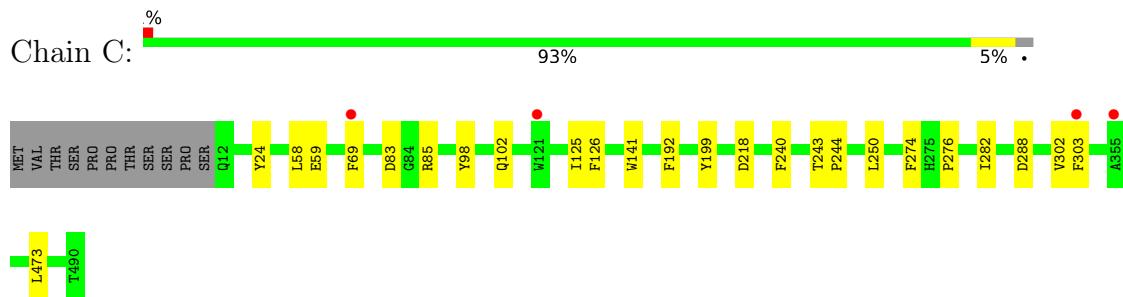
- Molecule 1: Apocarotenoid-15,15'-oxygenase



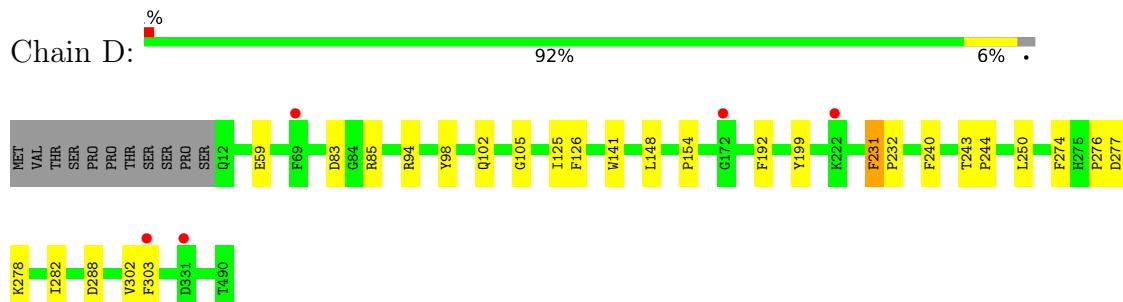
- Molecule 1: Apocarotenoid-15,15'-oxygenase



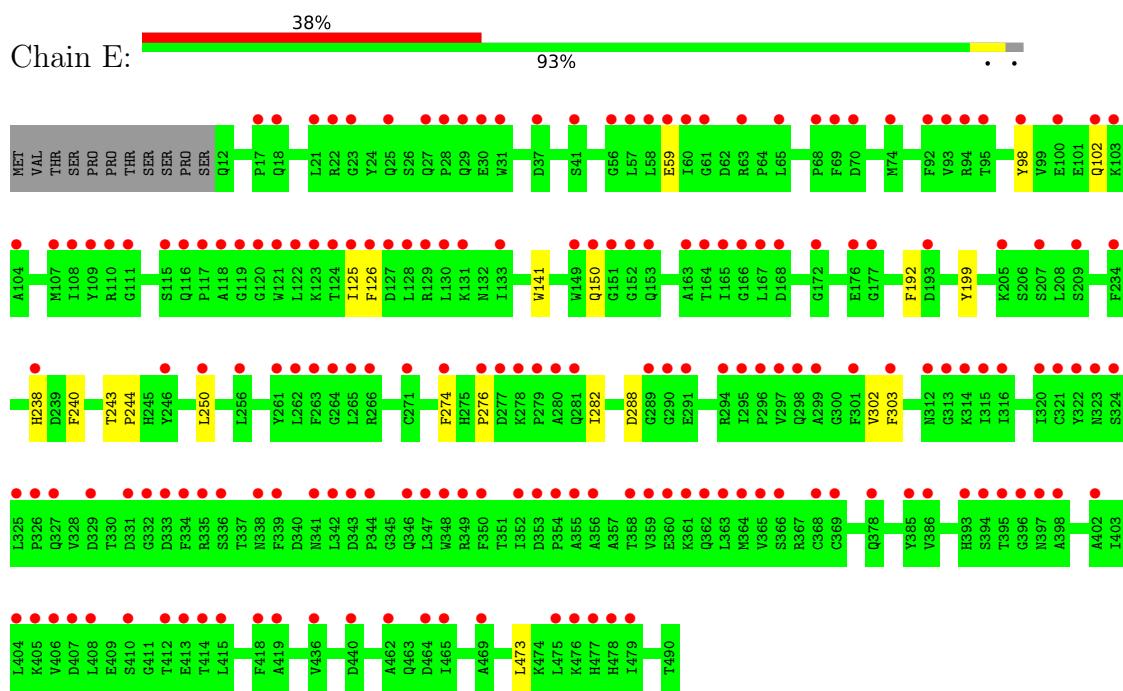
- Molecule 1: Apocarotenoid-15,15'-oxygenase



- Molecule 1: Apocarotenoid-15,15'-oxygenase



- Molecule 1: Apocarotenoid-15,15'-oxygenase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.53 Å 125.50 Å 203.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.42 – 2.75 46.77 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.42-2.75) 95.1 (46.77-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.68 (at 2.77 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R , R_{free}	0.212 , 0.247 0.216 , 0.249	Depositor DCC
R_{free} test set	3560 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.6	EDS
L-test for twinning ²	$< L > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18952	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

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	0.58	0/3881	0.66	0/5285
1	B	0.60	0/3881	0.66	0/5285
1	C	0.57	1/3881 (0.0%)	0.65	0/5285
1	D	0.56	0/3881	0.65	0/5285
1	E	0.41	0/3881	0.61	0/5285
All	All	0.55	1/19405 (0.0%)	0.64	0/26425

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	69	PHE	CG-CD2	5.30	1.46	1.38

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	3768	0	3661	20	0
1	B	3768	0	3661	20	0
1	C	3768	0	3661	20	0
1	D	3768	0	3661	23	0
1	E	3768	0	3661	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	33	0	0	2	0
3	B	29	0	0	2	0
3	C	25	0	0	0	0
3	D	18	0	0	0	0
3	E	2	0	0	0	0
All	All	18952	0	18305	94	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 3.

All (94) 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:C:274:PHE:CE2	1:C:276:PRO:HB3	2.16	0.81
1:D:274:PHE:CE2	1:D:276:PRO:HB3	2.16	0.81
1:E:250:LEU:HD23	1:E:302:VAL:HB	1.64	0.79
1:D:250:LEU:HD23	1:D:302:VAL:HB	1.64	0.78
1:D:274:PHE:CZ	1:D:276:PRO:HA	2.18	0.78
1:C:274:PHE:CZ	1:C:276:PRO:HA	2.19	0.77
1:E:274:PHE:CE2	1:E:276:PRO:HB3	2.19	0.77
1:B:250:LEU:HD23	1:B:302:VAL:HB	1.65	0.77
1:C:250:LEU:HD23	1:C:302:VAL:HB	1.69	0.75
1:E:274:PHE:CZ	1:E:276:PRO:HA	2.22	0.75
1:B:239:ASP:OD2	3:B:601:HOH:O	2.07	0.72
1:A:250:LEU:HD12	1:A:305:HIS:HE1	1.54	0.71
1:A:67:HIS:HE1	1:A:69:PHE:CD1	2.12	0.67
1:A:250:LEU:CD1	1:A:302:VAL:HG11	2.28	0.62
1:D:231:PHE:CD2	1:D:232:PRO:HD2	2.38	0.59
1:D:250:LEU:HD23	1:D:302:VAL:CB	2.33	0.57
1:B:250:LEU:HD23	1:B:302:VAL:CB	2.34	0.57
1:E:250:LEU:HD23	1:E:302:VAL:CB	2.34	0.56
1:A:67:HIS:CE1	1:A:69:PHE:CD1	2.93	0.55
1:E:150:GLN:OE1	1:E:238:HIS:CD2	2.60	0.54
1:D:277:ASP:OD1	1:D:278:LYS:N	2.40	0.54
1:D:231:PHE:CE1	1:D:232:PRO:O	2.60	0.54
1:E:250:LEU:HD12	1:E:282:ILE:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:VAL:HG12	1:B:274:PHE:CD1	2.43	0.53
1:B:250:LEU:HD11	1:B:282:ILE:HG12	1.91	0.53
1:C:250:LEU:HD23	1:C:302:VAL:CB	2.37	0.52
1:B:250:LEU:HD12	1:B:282:ILE:HA	1.92	0.52
1:D:250:LEU:HD11	1:D:282:ILE:HG12	1.93	0.51
1:E:250:LEU:HD11	1:E:282:ILE:HG12	1.91	0.51
1:C:250:LEU:HD12	1:C:282:ILE:HA	1.92	0.51
1:C:250:LEU:HD11	1:C:282:ILE:HG12	1.93	0.51
1:A:254:VAL:HG12	1:A:274:PHE:CD1	2.45	0.51
1:A:90:SER:OG	3:A:601:HOH:O	2.19	0.50
1:C:125:ILE:HG12	1:C:126:PHE:CD2	2.47	0.50
1:B:125:ILE:HG12	1:B:126:PHE:CD2	2.47	0.50
1:D:274:PHE:CZ	1:D:276:PRO:CA	2.93	0.50
1:D:250:LEU:HD12	1:D:282:ILE:HA	1.93	0.49
1:B:67:HIS:CD2	1:B:69:PHE:HB2	2.47	0.49
1:D:125:ILE:HG12	1:D:126:PHE:CD2	2.48	0.49
1:A:125:ILE:HG12	1:A:126:PHE:CD2	2.49	0.48
1:B:67:HIS:HD2	1:B:69:PHE:HB2	1.80	0.47
1:A:141:TRP:CE2	1:A:199:TYR:HB2	2.50	0.47
1:B:250:LEU:CD1	1:B:282:ILE:HG12	2.45	0.47
1:E:125:ILE:HG12	1:E:126:PHE:CD2	2.49	0.47
1:A:473:LEU:HD12	1:A:473:LEU:N	2.30	0.46
1:E:250:LEU:CD1	1:E:282:ILE:HG12	2.45	0.46
1:C:274:PHE:CZ	1:C:276:PRO:CA	2.94	0.46
1:B:243:THR:HB	1:B:244:PRO:CD	2.47	0.45
1:D:250:LEU:CD1	1:D:282:ILE:HG12	2.46	0.45
1:A:243:THR:HB	1:A:244:PRO:CD	2.47	0.45
1:D:192:PHE:CE1	1:D:288:ASP:HB3	2.51	0.45
1:E:274:PHE:CZ	1:E:276:PRO:CA	2.97	0.45
1:C:250:LEU:CD1	1:C:282:ILE:HG12	2.47	0.45
1:B:18:GLN:HB3	1:D:102:GLN:OE1	2.17	0.44
1:C:243:THR:HB	1:C:244:PRO:CD	2.47	0.44
1:A:192:PHE:CE1	1:A:288:ASP:HB3	2.52	0.44
1:A:473:LEU:N	1:A:473:LEU:CD1	2.80	0.44
1:D:243:THR:HB	1:D:244:PRO:CD	2.47	0.44
1:E:192:PHE:CE1	1:E:288:ASP:HB3	2.53	0.44
1:C:98:TYR:O	1:C:102:GLN:HG2	2.17	0.44
1:A:95:THR:OG1	3:A:602:HOH:O	2.21	0.43
1:A:480:PRO:O	1:A:481:TYR:C	2.57	0.43
1:B:22:ARG:NH2	1:D:105:GLY:HA2	2.34	0.43
1:D:250:LEU:CD2	1:D:302:VAL:HG21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:LEU:CD2	1:E:302:VAL:HG21	2.48	0.42
1:D:98:TYR:O	1:D:102:GLN:HG2	2.19	0.42
1:B:235:ALA:HA	3:B:625:HOH:O	2.19	0.42
1:C:192:PHE:CE1	1:C:288:ASP:HB3	2.55	0.42
1:E:141:TRP:CE2	1:E:199:TYR:HB2	2.54	0.42
1:A:243:THR:HB	1:A:244:PRO:HD2	2.02	0.42
1:B:192:PHE:CE1	1:B:288:ASP:HB3	2.55	0.42
1:B:243:THR:HB	1:B:244:PRO:HD2	2.02	0.42
1:D:243:THR:HB	1:D:244:PRO:HD2	2.02	0.41
1:C:243:THR:HB	1:C:244:PRO:HD2	2.03	0.41
1:C:141:TRP:CE2	1:C:199:TYR:HB2	2.56	0.41
1:D:141:TRP:CE2	1:D:199:TYR:HB2	2.55	0.41
1:E:473:LEU:HD12	1:E:473:LEU:N	2.35	0.41
1:B:22:ARG:NE	1:D:102:GLN:O	2.46	0.41
1:B:250:LEU:CD2	1:B:302:VAL:HG21	2.51	0.41
1:C:473:LEU:N	1:C:473:LEU:HD12	2.35	0.41
1:D:83:ASP:OD1	1:D:85:ARG:HB2	2.21	0.41
1:A:277:ASP:OD2	1:B:476:LYS:NZ	2.44	0.41
1:A:375:HIS:HD2	1:A:438:GLU:O	2.04	0.41
1:C:250:LEU:CD2	1:C:302:VAL:HG21	2.50	0.41
1:E:243:THR:HB	1:E:244:PRO:CD	2.50	0.41
1:C:218:ASP:OD1	1:C:218:ASP:C	2.60	0.40
1:A:218:ASP:C	1:A:218:ASP:OD1	2.60	0.40
1:A:250:LEU:HD21	1:A:282:ILE:HG12	2.03	0.40
1:B:141:TRP:CE2	1:B:199:TYR:HB2	2.57	0.40
1:D:148:LEU:HD23	1:D:154:PRO:HB3	2.03	0.40
1:E:98:TYR:O	1:E:102:GLN:HG2	2.21	0.40
1:C:24:TYR:O	1:C:58:LEU:HD13	2.21	0.40
1:A:18:GLN:HG2	1:C:102:GLN:OE1	2.21	0.40
1:C:83:ASP:OD1	1:C:85:ARG:HB2	2.21	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	477/490 (97%)	461 (97%)	16 (3%)	0	100	100
1	B	477/490 (97%)	459 (96%)	18 (4%)	0	100	100
1	C	477/490 (97%)	460 (96%)	17 (4%)	0	100	100
1	D	477/490 (97%)	459 (96%)	18 (4%)	0	100	100
1	E	477/490 (97%)	461 (97%)	16 (3%)	0	100	100
All	All	2385/2450 (97%)	2300 (96%)	85 (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	399/410 (97%)	396 (99%)	3 (1%)	81	88
1	B	399/410 (97%)	396 (99%)	3 (1%)	81	88
1	C	399/410 (97%)	396 (99%)	3 (1%)	81	88
1	D	399/410 (97%)	394 (99%)	5 (1%)	69	81
1	E	399/410 (97%)	396 (99%)	3 (1%)	81	88
All	All	1995/2050 (97%)	1978 (99%)	17 (1%)	78	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	240	PHE
1	A	303	PHE
1	B	59	GLU
1	B	240	PHE
1	B	303	PHE
1	C	59	GLU

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Mol	Chain	Res	Type
1	C	240	PHE
1	C	303	PHE
1	D	59	GLU
1	D	94	ARG
1	D	231	PHE
1	D	240	PHE
1	D	303	PHE
1	E	59	GLU
1	E	240	PHE
1	E	303	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	150	GLN
1	B	150	GLN
1	C	150	GLN
1	C	275	HIS
1	D	150	GLN
1	E	150	GLN
1	E	238	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	479/490 (97%)	-0.34	5 (1%)	82	87	29, 49, 90, 141
1	B	479/490 (97%)	-0.25	3 (0%)	89	92	28, 49, 81, 132
1	C	479/490 (97%)	-0.24	4 (0%)	86	90	28, 52, 96, 125
1	D	479/490 (97%)	-0.19	5 (1%)	82	87	32, 57, 95, 128
1	E	479/490 (97%)	1.82	185 (38%)	0	0	80, 128, 171, 223
All	All	2395/2450 (97%)	0.16	202 (8%)	11	13	28, 57, 144, 223

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	263	PHE	12.3
1	E	121	TRP	9.8
1	E	120	GLY	9.6
1	E	122	LEU	7.9
1	E	125	ILE	7.8
1	E	277	ASP	7.0
1	E	331	ASP	6.8
1	E	118	ALA	6.4
1	E	119	GLY	6.4
1	E	98	TYR	6.3
1	E	359	VAL	6.3
1	E	281	GLN	6.2
1	E	124	THR	6.1
1	E	274	PHE	6.1
1	E	348	TRP	6.0
1	E	126	PHE	5.9
1	E	279	PRO	5.8
1	E	296	PRO	5.5
1	E	462	ALA	5.1
1	E	333	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	130	LEU	5.0
1	E	344	PRO	4.9
1	E	476	LYS	4.9
1	E	265	LEU	4.8
1	E	341	ASN	4.8
1	E	264	GLY	4.7
1	E	18	GLN	4.5
1	E	334	PHE	4.5
1	E	298	GLN	4.4
1	E	299	ALA	4.4
1	E	396	GLY	4.4
1	E	61	GLY	4.4
1	E	58	LEU	4.4
1	E	60	ILE	4.4
1	E	355	ALA	4.4
1	E	261	TYR	4.3
1	E	350	PHE	4.3
1	E	342	LEU	4.2
1	E	94	ARG	4.2
1	E	276	PRO	4.2
1	E	338	ASN	4.1
1	E	266	ARG	4.1
1	E	128	LEU	4.1
1	E	356	ALA	4.1
1	E	393	HIS	4.0
1	E	256	LEU	4.0
1	E	343	ASP	4.0
1	E	436	VAL	4.0
1	E	93	VAL	3.9
1	E	332	GLY	3.9
1	E	323	ASN	3.9
1	C	303	PHE	3.9
1	E	418	PHE	3.9
1	E	131	LYS	3.8
1	E	289	GLY	3.8
1	E	397	ASN	3.8
1	E	312	ASN	3.7
1	E	405	LYS	3.7
1	E	415	LEU	3.7
1	E	163	ALA	3.7
1	E	100	GLU	3.6
1	E	21	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	354	PRO	3.6
1	E	297	VAL	3.6
1	E	294	ARG	3.5
1	E	413	GLU	3.5
1	E	295	ILE	3.5
1	E	315	ILE	3.5
1	E	398	ALA	3.5
1	E	464	ASP	3.4
1	E	404	LEU	3.4
1	E	262	LEU	3.4
1	E	325	LEU	3.4
1	E	123	LYS	3.4
1	E	362	GLN	3.4
1	E	69	PHE	3.4
1	E	347	LEU	3.4
1	E	313	GLY	3.4
1	E	465	ILE	3.4
1	E	56	GLY	3.4
1	E	176	GLU	3.3
1	E	329	ASP	3.3
1	E	419	ALA	3.3
1	E	352	ILE	3.3
1	E	395	THR	3.3
1	E	234	PHE	3.3
1	E	109	TYR	3.3
1	E	477	HIS	3.3
1	E	166	GLY	3.3
1	E	402	ALA	3.2
1	E	110	ARG	3.2
1	E	314	LYS	3.2
1	E	238	HIS	3.2
1	E	394	SER	3.1
1	E	68	PRO	3.1
1	E	368	CYS	3.1
1	E	116	GLN	3.1
1	E	167	LEU	3.1
1	E	475	LEU	3.1
1	E	102	GLN	3.1
1	E	207	SER	3.0
1	E	65	LEU	3.0
1	E	303	PHE	3.0
1	E	107	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	193	ASP	3.0
1	A	69	PHE	3.0
1	E	339	PHE	3.0
1	E	414	THR	3.0
1	E	27	GLN	2.9
1	E	152	GLY	2.9
1	E	165	ILE	2.9
1	E	478	HIS	2.9
1	E	30	GLU	2.9
1	E	129	ARG	2.9
1	E	316	ILE	2.9
1	E	25	GLN	2.8
1	E	291	GLU	2.8
1	E	440	ASP	2.8
1	E	327	GLN	2.8
1	E	57	LEU	2.8
1	E	410	SER	2.8
1	A	121	TRP	2.8
1	E	172	GLY	2.8
1	E	149	TRP	2.7
1	E	22	ARG	2.7
1	E	153	GLN	2.7
1	E	17	PRO	2.7
1	E	349	ARG	2.7
1	E	385	TYR	2.7
1	B	69	PHE	2.7
1	E	346	GLN	2.7
1	E	127	ASP	2.7
1	E	364	MET	2.6
1	E	407	ASP	2.6
1	E	205	LYS	2.6
1	E	301	PHE	2.6
1	E	104	ALA	2.6
1	C	69	PHE	2.6
1	E	335	ARG	2.6
1	E	92	PHE	2.6
1	E	95	THR	2.6
1	E	360	GLU	2.5
1	E	336	SER	2.5
1	E	324	SER	2.5
1	E	59	GLU	2.5
1	A	303	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	28	PRO	2.5
1	E	74	MET	2.5
1	E	164	THR	2.5
1	D	303	PHE	2.5
1	E	290	GLY	2.5
1	E	150	GLN	2.5
1	E	108	ILE	2.4
1	E	321	CYS	2.4
1	E	412	THR	2.4
1	E	408	LEU	2.4
1	E	117	PRO	2.4
1	E	479	ILE	2.4
1	E	406	VAL	2.4
1	E	278	LYS	2.4
1	E	115	SER	2.4
1	E	103	LYS	2.4
1	E	133	ILE	2.3
1	A	208	LEU	2.3
1	B	303	PHE	2.3
1	E	378	GLN	2.3
1	B	121	TRP	2.3
1	D	69	PHE	2.3
1	E	209	SER	2.3
1	A	274	PHE	2.3
1	E	369	CYS	2.3
1	E	41	SER	2.2
1	E	322	TYR	2.2
1	E	111	GLY	2.2
1	E	151	GLY	2.2
1	E	386	VAL	2.2
1	D	331	ASP	2.2
1	E	168	ASP	2.2
1	D	222	LYS	2.2
1	E	365	VAL	2.2
1	E	363	LEU	2.2
1	E	469	ALA	2.2
1	E	320	ILE	2.2
1	E	361	LYS	2.1
1	E	29	GLN	2.1
1	E	326	PRO	2.1
1	E	63	ARG	2.1
1	E	358	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	31	TRP	2.1
1	C	121	TRP	2.1
1	E	366	SER	2.1
1	E	271	CYS	2.1
1	C	355	ALA	2.1
1	E	280	ALA	2.1
1	E	37	ASP	2.1
1	E	177	GLY	2.1
1	E	353	ASP	2.1
1	E	250	LEU	2.0
1	E	246	TYR	2.0
1	E	70	ASP	2.0
1	E	23	GLY	2.0
1	D	172	GLY	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 monosaccharides 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	FE2	E	501	1/1	0.41	0.33	155,155,155,155	0
2	FE2	B	501	1/1	0.93	0.10	62,62,62,62	0
2	FE2	C	501	1/1	0.94	0.10	75,75,75,75	0
2	FE2	A	501	1/1	0.96	0.09	75,75,75,75	0
2	FE2	D	501	1/1	0.98	0.14	74,74,74,74	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.