



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2017 – 05:39 AM EDT

PDB ID : 5KJA  
Title : Synechocystis apocarotenoid oxygenase (ACO) mutant - Trp149Ala  
Authors : Sui, X.; Kiser, P.D.; Palczewski, K.  
Deposited on : unknown  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029824

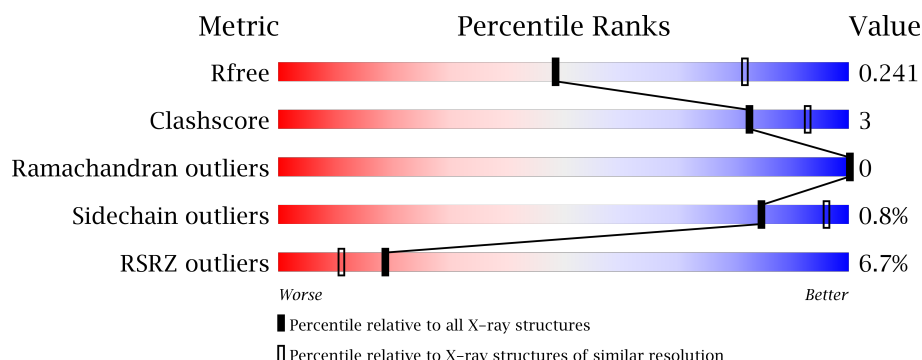
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	490	<div> <div>91%</div> <div>7%</div> </div>
1	B	490	<div> <div>91%</div> <div>7%</div> </div>
1	C	490	<div> <div>90%</div> <div>8%</div> </div>
1	D	490	<div> <div>90%</div> <div>7%</div> </div>
1	E	490	<div> <div>32%</div> <div>91%</div> <div>7%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18975 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	482	Total	C	N	O	S	0	0	0
			3778	2420	652	696	10			
1	B	479	Total	C	N	O	S	0	0	0
			3759	2409	649	691	10			
1	C	479	Total	C	N	O	S	0	0	0
			3759	2409	649	691	10			
1	D	479	Total	C	N	O	S	0	0	0
			3759	2409	649	691	10			
1	E	479	Total	C	N	O	S	0	0	0
			3759	2409	649	691	10			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	ALA	TRP	engineered mutation	UNP P74334
B	149	ALA	TRP	engineered mutation	UNP P74334
C	149	ALA	TRP	engineered mutation	UNP P74334
D	149	ALA	TRP	engineered mutation	UNP P74334
E	149	ALA	TRP	engineered mutation	UNP P74334

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

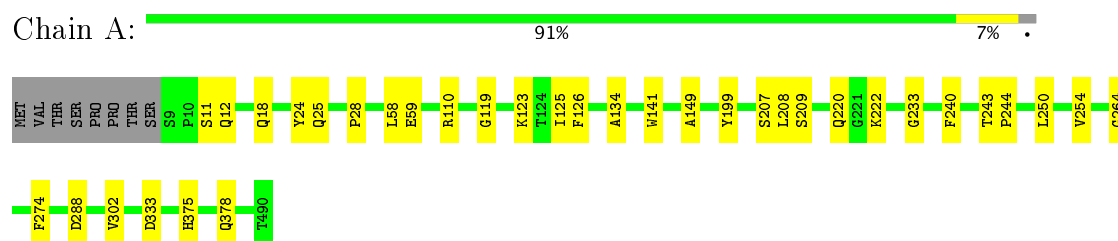
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	49	Total O 49 49	0	0
4	B	39	Total O 39 39	0	0
4	C	39	Total O 39 39	0	0
4	D	26	Total O 26 26	0	0
4	E	1	Total O 1 1	0	0

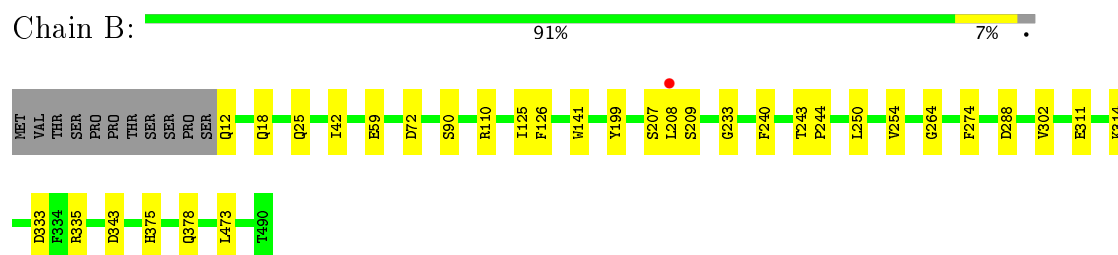
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

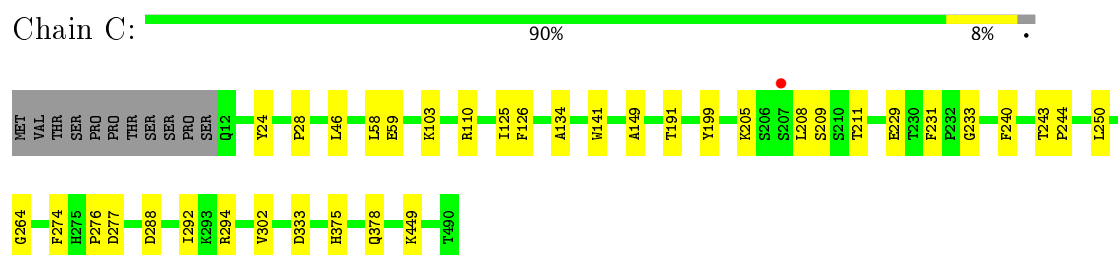
#### • Molecule 1: Apocarotenoid-15,15'-oxygenase



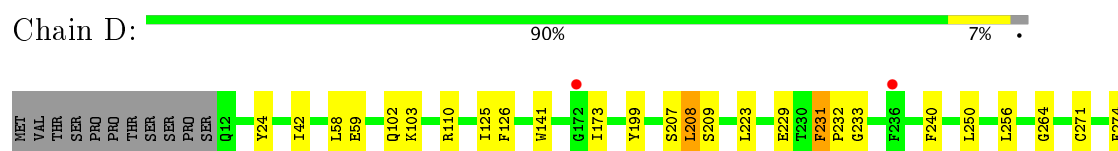
#### • Molecule 1: Apocarotenoid-15,15'-oxygenase



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

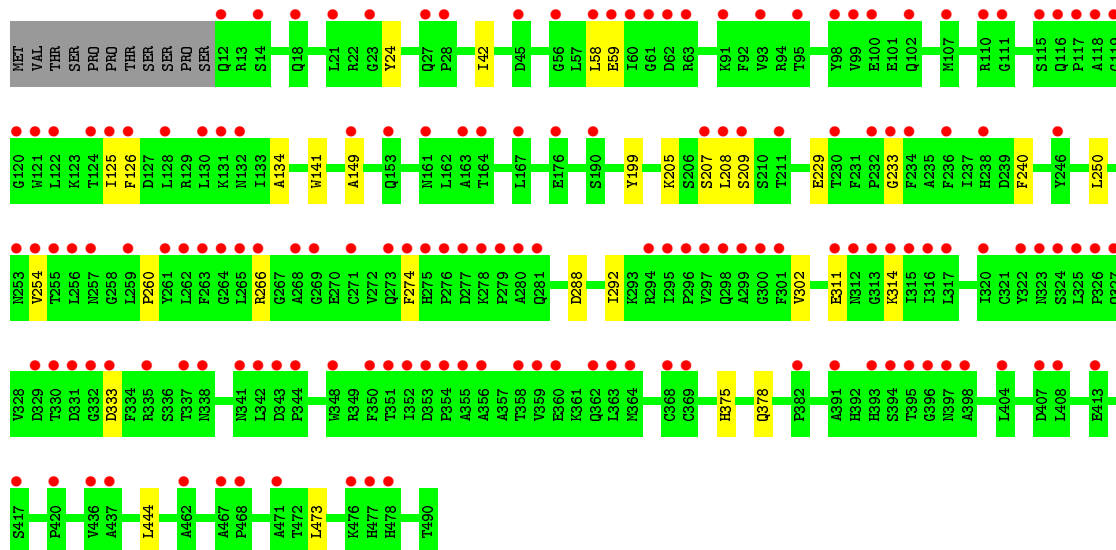
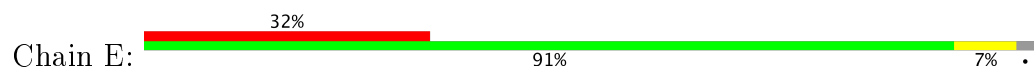


#### • Molecule 1: Apocarotenoid-15,15'-oxygenase





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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.14Å 125.26Å 203.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.62 – 2.80 47.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.62-2.80) 100.0 (47.31-2.80)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.198 , 0.239 0.203 , 0.241	Depositor DCC
$R_{free}$ test set	3595 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.7	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, 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	0.63	0/3890	0.72	2/5297 (0.0%)
1	B	0.61	0/3870	0.71	2/5269 (0.0%)
1	C	0.60	0/3870	0.71	2/5269 (0.0%)
1	D	0.59	0/3870	0.71	2/5269 (0.0%)
1	E	0.45	0/3870	0.66	3/5269 (0.1%)
All	All	0.58	0/19370	0.70	11/26373 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	288	ASP	CB-CG-OD1	6.93	124.53	118.30
1	D	288	ASP	CB-CG-OD2	6.77	124.39	118.30
1	E	288	ASP	CB-CG-OD1	6.46	124.11	118.30
1	B	288	ASP	CB-CG-OD1	6.33	124.00	118.30
1	E	444	LEU	CB-CG-CD1	6.29	121.70	111.00
1	A	288	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	D	288	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	E	288	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	C	288	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	B	288	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	C	288	ASP	CB-CG-OD2	5.27	123.05	118.30

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	3778	0	3671	20	0
1	B	3759	0	3654	21	0
1	C	3759	0	3654	30	1
1	D	3759	0	3654	28	0
1	E	3759	0	3654	15	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	49	0	0	0	0
4	B	39	0	0	3	0
4	C	39	0	0	3	0
4	D	26	0	0	1	0
4	E	1	0	0	0	0
All	All	18975	0	18287	109	1

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 (109) 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:291:GLU:HA	4:D:624:HOH:O	1.65	0.97
1:C:229:GLU:HG3	1:C:292:ILE:HD11	1.65	0.79
1:A:119:GLY:HA3	1:A:123:LYS:HG3	1.64	0.78
1:D:229:GLU:HG3	1:D:292:ILE:HD11	1.68	0.75
1:E:254:VAL:HG22	1:E:274:PHE:CD1	2.30	0.67
1:A:119:GLY:HA3	1:A:123:LYS:CG	2.25	0.66
1:A:208:LEU:O	1:A:233:GLY:N	2.28	0.66
1:D:231:PHE:CE2	1:D:232:PRO:O	2.48	0.66
1:B:254:VAL:HG12	1:B:274:PHE:CD1	2.31	0.66
1:D:208:LEU:O	1:D:233:GLY:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:HG22	1:A:274:PHE:CD1	2.32	0.64
1:C:208:LEU:O	1:C:233:GLY:N	2.30	0.64
1:E:208:LEU:O	1:E:233:GLY:N	2.31	0.63
1:C:205:LYS:HG2	1:C:205:LYS:O	1.99	0.62
1:C:449:LYS:HD2	4:C:625:HOH:O	2.00	0.62
1:A:220:GLN:HB3	1:A:222:LYS:HE3	1.82	0.61
1:B:208:LEU:O	1:B:233:GLY:N	2.29	0.61
1:A:220:GLN:CB	1:A:222:LYS:HE3	2.33	0.59
1:B:18:GLN:CG	1:D:102:GLN:OE1	2.52	0.58
1:C:205:LYS:CG	1:C:205:LYS:O	2.53	0.57
1:C:125:ILE:HG12	1:C:126:PHE:CD2	2.41	0.56
1:C:229:GLU:HG3	1:C:292:ILE:CD1	2.36	0.54
1:D:125:ILE:HG12	1:D:126:PHE:CD2	2.43	0.54
1:E:254:VAL:CG2	1:E:274:PHE:CD1	2.90	0.54
1:A:25:GLN:OE1	1:C:103:LYS:HG2	2.08	0.53
1:B:125:ILE:HG12	1:B:126:PHE:CD2	2.43	0.53
1:A:125:ILE:HG12	1:A:126:PHE:CD2	2.44	0.53
1:B:25:GLN:OE1	1:D:103:LYS:HG2	2.09	0.53
1:E:125:ILE:HG12	1:E:126:PHE:CD2	2.44	0.53
1:A:254:VAL:CG2	1:A:274:PHE:CD1	2.93	0.52
1:D:231:PHE:CZ	1:D:232:PRO:O	2.64	0.51
1:D:229:GLU:HG3	1:D:292:ILE:CD1	2.38	0.51
1:B:90:SER:OG	4:B:601:HOH:O	2.12	0.50
1:E:250:LEU:HD22	1:E:302:VAL:HB	1.95	0.48
1:C:110:ARG:NH2	1:C:264:GLY:HA2	2.29	0.48
1:D:173:ILE:HG23	1:D:223:LEU:HD12	1.95	0.48
1:D:250:LEU:HD22	1:D:302:VAL:HB	1.96	0.48
1:D:250:LEU:HD23	1:D:250:LEU:C	2.33	0.48
1:C:229:GLU:CD	1:C:292:ILE:CD1	2.83	0.47
1:B:72:ASP:HB3	4:B:617:HOH:O	2.14	0.47
1:D:375:HIS:HB3	1:D:378:GLN:HG2	1.97	0.47
1:C:229:GLU:CG	1:C:292:ILE:CD1	2.93	0.46
1:C:274:PHE:CZ	1:C:276:PRO:HB3	2.50	0.46
1:D:333:ASP:C	1:D:333:ASP:OD1	2.54	0.46
1:B:250:LEU:HD22	1:B:302:VAL:HB	1.98	0.46
1:B:333:ASP:OD1	1:B:333:ASP:C	2.54	0.45
1:C:229:GLU:CD	1:C:292:ILE:HD12	2.37	0.45
1:A:243:THR:HB	1:A:244:PRO:CD	2.47	0.45
1:B:207:SER:HB2	1:B:209:SER:H	1.82	0.45
1:E:375:HIS:HB3	1:E:378:GLN:HG2	1.98	0.45
1:A:333:ASP:C	1:A:333:ASP:OD1	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLN:HG2	1:D:102:GLN:OE1	2.16	0.45
1:A:141:TRP:CE2	1:A:199:TYR:HB2	2.52	0.45
1:C:141:TRP:CE2	1:C:199:TYR:HB2	2.52	0.44
1:C:277:ASP:OD1	1:C:277:ASP:N	2.51	0.44
1:C:250:LEU:HD22	1:C:302:VAL:HB	1.98	0.44
1:E:42:ILE:HD11	1:E:473:LEU:HD21	2.00	0.44
1:A:243:THR:HB	1:A:244:PRO:HD2	2.00	0.44
1:C:375:HIS:HB3	1:C:378:GLN:HG2	2.00	0.44
1:B:141:TRP:CE2	1:B:199:TYR:HB2	2.52	0.44
1:C:46:LEU:O	4:C:601:HOH:O	2.21	0.44
1:C:231:PHE:HB3	1:C:294:ARG:NH2	2.33	0.44
1:D:229:GLU:CD	1:D:292:ILE:CD1	2.86	0.44
1:C:205:LYS:HE3	1:C:211:THR:HB	2.00	0.44
1:A:207:SER:HB2	1:A:209:SER:H	1.83	0.43
1:A:250:LEU:HD22	1:A:302:VAL:HB	1.99	0.43
1:C:333:ASP:C	1:C:333:ASP:OD1	2.56	0.43
1:D:274:PHE:CZ	1:D:276:PRO:HB3	2.53	0.43
1:B:250:LEU:HD23	1:B:250:LEU:C	2.39	0.43
1:E:333:ASP:OD1	1:E:333:ASP:C	2.57	0.43
1:C:243:THR:HB	1:C:244:PRO:CD	2.48	0.43
1:C:231:PHE:CB	1:C:294:ARG:NH2	2.82	0.43
1:D:277:ASP:OD1	1:D:277:ASP:N	2.51	0.43
1:D:42:ILE:HD11	1:D:473:LEU:HD21	2.01	0.42
1:B:110:ARG:NH2	1:B:264:GLY:HA2	2.35	0.42
1:C:191:THR:HG22	4:C:617:HOH:O	2.19	0.42
1:C:229:GLU:CG	1:C:292:ILE:HD11	2.41	0.42
1:D:229:GLU:CD	1:D:292:ILE:HD12	2.40	0.42
1:E:207:SER:HB2	1:E:209:SER:H	1.85	0.42
1:D:231:PHE:CD2	1:D:232:PRO:O	2.72	0.42
1:B:343:ASP:HB3	4:B:636:HOH:O	2.19	0.42
1:C:24:TYR:O	1:C:58:LEU:HD13	2.20	0.42
1:D:311:GLU:O	1:D:314:LYS:HB2	2.20	0.42
1:A:375:HIS:HB3	1:A:378:GLN:HG2	2.02	0.42
1:D:229:GLU:CG	1:D:292:ILE:CD1	2.97	0.42
1:B:375:HIS:HB3	1:B:378:GLN:HG2	2.01	0.41
1:C:250:LEU:HD23	1:C:250:LEU:C	2.40	0.41
1:D:207:SER:HB2	1:D:209:SER:H	1.84	0.41
1:A:18:GLN:HE22	1:C:28:PRO:CB	2.33	0.41
1:E:141:TRP:CE2	1:E:199:TYR:HB2	2.56	0.41
1:A:134:ALA:HA	1:A:149:ALA:HB2	2.03	0.41
1:E:134:ALA:HA	1:E:149:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLU:O	1:B:314:LYS:HB2	2.20	0.41
1:D:24:TYR:O	1:D:58:LEU:HD13	2.20	0.41
1:B:42:ILE:HD11	1:B:473:LEU:HD21	2.02	0.41
1:D:141:TRP:CE2	1:D:199:TYR:HB2	2.56	0.41
1:B:243:THR:HB	1:B:244:PRO:HD2	2.02	0.41
1:E:229:GLU:HG2	1:E:292:ILE:HD13	2.03	0.41
1:B:333:ASP:OD2	1:B:335:ARG:NH1	2.53	0.41
1:D:256:LEU:HD12	1:D:271:CYS:O	2.21	0.41
1:A:110:ARG:NH2	1:A:264:GLY:HA2	2.36	0.41
1:E:260:PRO:HB2	1:E:266:ARG:HG2	2.03	0.41
1:A:24:TYR:O	1:A:58:LEU:HD13	2.20	0.40
1:B:243:THR:HB	1:B:244:PRO:CD	2.50	0.40
1:E:311:GLU:O	1:E:314:LYS:HB2	2.21	0.40
1:C:134:ALA:HA	1:C:149:ALA:HB2	2.04	0.40
1:C:243:THR:HB	1:C:244:PRO:HD2	2.02	0.40
1:E:24:TYR:O	1:E:58:LEU:HD13	2.21	0.40
1:D:110:ARG:NH2	1:D:264:GLY:HA2	2.35	0.40

All (1) 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:C:209:SER:OG	1:E:205:LYS:NZ[2_545]	2.11	0.09

## 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	480/490 (98%)	466 (97%)	14 (3%)	0	100	100
1	B	477/490 (97%)	463 (97%)	14 (3%)	0	100	100
1	C	477/490 (97%)	462 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	477/490 (97%)	463 (97%)	14 (3%)	0	100	100
1	E	477/490 (97%)	463 (97%)	14 (3%)	0	100	100
All	All	2388/2450 (98%)	2317 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	401/409 (98%)	396 (99%)	5 (1%)	75	94
1	B	398/409 (97%)	395 (99%)	3 (1%)	85	96
1	C	398/409 (97%)	396 (100%)	2 (0%)	91	97
1	D	398/409 (97%)	394 (99%)	4 (1%)	80	95
1	E	398/409 (97%)	396 (100%)	2 (0%)	91	97
All	All	1993/2045 (98%)	1977 (99%)	16 (1%)	85	96

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	12	GLN
1	A	28	PRO
1	A	59	GLU
1	A	240	PHE
1	B	12	GLN
1	B	59	GLU
1	B	240	PHE
1	C	59	GLU
1	C	240	PHE
1	D	59	GLU
1	D	208	LEU
1	D	231	PHE

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Mol	Chain	Res	Type
1	D	240	PHE
1	E	59	GLU
1	E	240	PHE

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 ⓘ

Of 7 ligands modelled in this entry, 7 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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	482/490 (98%)	-0.42	0 100 100	31, 55, 94, 144	0
1	B	479/490 (97%)	-0.33	1 (0%) 94 94	34, 56, 94, 132	0
1	C	479/490 (97%)	-0.35	1 (0%) 94 94	34, 57, 97, 177	0
1	D	479/490 (97%)	-0.29	2 (0%) 92 90	36, 63, 107, 168	0
1	E	479/490 (97%)	1.48	156 (32%) 0 0	81, 130, 185, 240	0
All	All	2398/2450 (97%)	0.02	160 (6%) 19 11	31, 63, 152, 240	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	263	PHE	8.6
1	E	124	THR	7.5
1	E	256	LEU	6.9
1	E	118	ALA	6.7
1	E	125	ILE	6.6
1	E	126	PHE	6.5
1	E	332	GLY	6.4
1	E	331	ASP	6.3
1	E	121	TRP	6.1
1	E	209	SER	5.6
1	E	348	TRP	5.4
1	E	333	ASP	5.4
1	E	266	ARG	5.1
1	E	234	PHE	5.1
1	E	313	GLY	5.1
1	E	276	PRO	4.8
1	E	56	GLY	4.7
1	E	299	ALA	4.7
1	E	100	GLU	4.7
1	E	279	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	300	GLY	4.6
1	E	262	LEU	4.5
1	E	393	HIS	4.5
1	E	232	PRO	4.3
1	E	230	THR	4.3
1	E	264	GLY	4.3
1	E	355	ALA	4.3
1	E	277	ASP	4.3
1	E	120	GLY	4.3
1	E	60	ILE	4.2
1	E	359	VAL	4.2
1	E	119	GLY	4.2
1	E	207	SER	4.1
1	E	58	LEU	4.1
1	E	261	TYR	4.0
1	E	323	ASN	4.0
1	E	298	GLN	3.8
1	E	360	GLU	3.8
1	E	102	GLN	3.8
1	E	271	CYS	3.8
1	E	208	LEU	3.8
1	E	236	PHE	3.8
1	E	269	GLY	3.7
1	E	344	PRO	3.7
1	E	343	ASP	3.7
1	E	274	PHE	3.7
1	E	257	ASN	3.7
1	E	259	LEU	3.6
1	E	476	LYS	3.6
1	E	12	GLN	3.6
1	E	398	ALA	3.5
1	E	329	ASP	3.4
1	E	107	MET	3.4
1	E	330	THR	3.4
1	E	176	GLU	3.4
1	E	397	ASN	3.4
1	E	297	VAL	3.3
1	E	273	GLN	3.3
1	E	275	HIS	3.2
1	E	327	GLN	3.2
1	E	255	THR	3.2
1	E	163	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	467	ALA	3.1
1	E	294	ARG	3.1
1	E	115	SER	3.1
1	E	59	GLU	3.1
1	E	396	GLY	3.1
1	E	314	LYS	3.1
1	E	233	GLY	3.1
1	E	395	THR	3.1
1	E	296	PRO	3.0
1	E	278	LYS	3.0
1	E	394	SER	3.0
1	E	98	TYR	3.0
1	E	268	ALA	3.0
1	E	462	ALA	3.0
1	E	254	VAL	3.0
1	E	320	ILE	3.0
1	E	338	ASN	3.0
1	E	111	GLY	2.9
1	E	122	LEU	2.9
1	E	281	GLN	2.9
1	E	27	GLN	2.9
1	E	478	HIS	2.9
1	E	382	PRO	2.9
1	E	362	GLN	2.8
1	E	117	PRO	2.8
1	E	238	HIS	2.8
1	E	312	ASN	2.8
1	E	363	LEU	2.8
1	E	62	ASP	2.8
1	E	356	ALA	2.8
1	E	341	ASN	2.7
1	E	301	PHE	2.7
1	E	353	ASP	2.7
1	E	93	VAL	2.7
1	E	342	LEU	2.7
1	E	350	PHE	2.7
1	E	404	LEU	2.7
1	E	316	ILE	2.6
1	E	211	THR	2.6
1	E	116	GLN	2.6
1	E	413	GLU	2.6
1	E	132	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	358	THR	2.6
1	E	369	CYS	2.6
1	E	110	ARG	2.5
1	E	18	GLN	2.5
1	E	477	HIS	2.5
1	E	91	LYS	2.5
1	C	207	SER	2.5
1	D	236	PHE	2.5
1	E	368	CYS	2.5
1	E	295	ILE	2.5
1	E	326	PRO	2.5
1	E	335	ARG	2.5
1	E	354	PRO	2.4
1	E	14	SER	2.4
1	E	95	THR	2.4
1	E	161	ASN	2.4
1	E	253	ASN	2.4
1	E	265	LEU	2.4
1	E	324	SER	2.4
1	E	317	LEU	2.4
1	E	391	ALA	2.4
1	E	130	LEU	2.4
1	E	128	LEU	2.3
1	E	311	GLU	2.3
1	B	208	LEU	2.3
1	E	337	THR	2.3
1	E	351	THR	2.3
1	E	471	ALA	2.3
1	E	21	LEU	2.2
1	E	164	THR	2.2
1	E	246	TYR	2.2
1	E	149	ALA	2.2
1	E	190	SER	2.2
1	E	315	ILE	2.2
1	E	417	SER	2.2
1	E	63	ARG	2.2
1	E	436	VAL	2.2
1	E	45	ASP	2.1
1	E	131	LYS	2.1
1	E	28	PRO	2.1
1	E	407	ASP	2.1
1	E	99	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	468	PRO	2.1
1	E	437	ALA	2.1
1	E	325	LEU	2.1
1	D	172	GLY	2.1
1	E	23	GLY	2.1
1	E	153	GLN	2.0
1	E	352	ILE	2.0
1	E	364	MET	2.0
1	E	420	PRO	2.0
1	E	167	LEU	2.0
1	E	408	LEU	2.0
1	E	280	ALA	2.0
1	E	61	GLY	2.0
1	E	322	TYR	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 carbohydrates 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. 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CL	A	501	1/1	0.96	0.14	-0.51	61,61,61,61	0
3	FE2	C	501	1/1	0.95	0.15	-0.88	91,91,91,91	0
3	FE2	E	501	1/1	0.81	0.14	-0.91	152,152,152,152	0
3	FE2	D	501	1/1	0.95	0.12	-1.69	96,96,96,96	0
3	FE2	B	502	1/1	0.86	0.11	-1.84	97,97,97,97	0
3	FE2	A	502	1/1	0.89	0.10	-2.05	96,96,96,96	0
2	CL	B	501	1/1	0.96	0.10	-3.14	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.