Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2016 – 04:29 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
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:

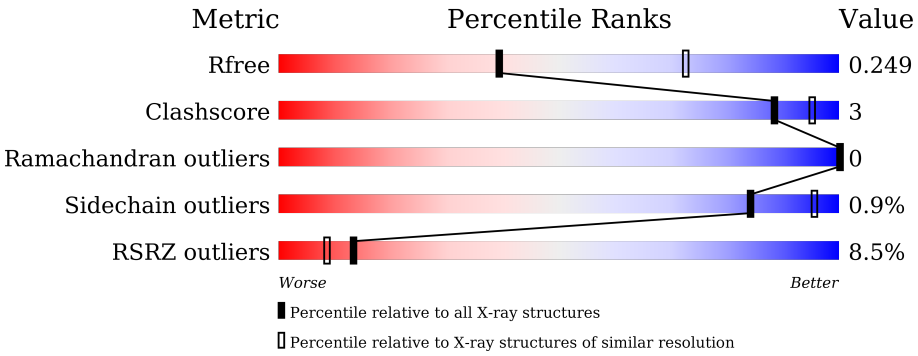
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.75 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}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	490	92% 6%
1	B	490	93% 5%
1	C	490	93% 5%
1	D	490	92% 6%
1	E	490	38% 93%

2 Entry composition

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	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

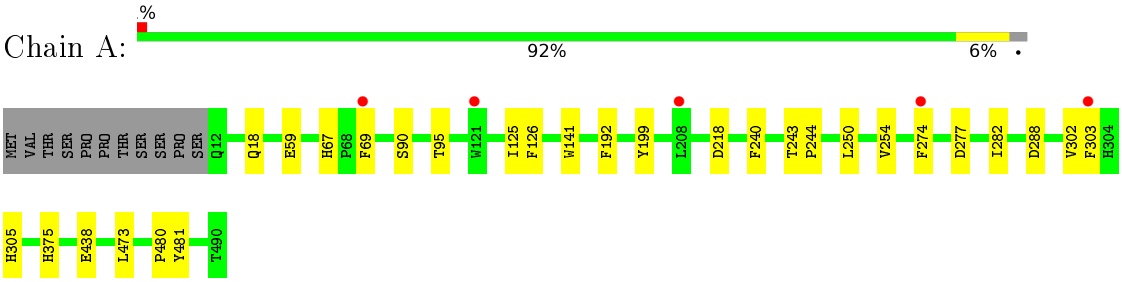
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	33	Total O 33 33	0	0
3	B	29	Total O 29 29	0	0
3	C	25	Total O 25 25	0	0
3	D	18	Total O 18 18	0	0
3	E	2	Total O 2 2	0	0

3 Residue-property plots (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.

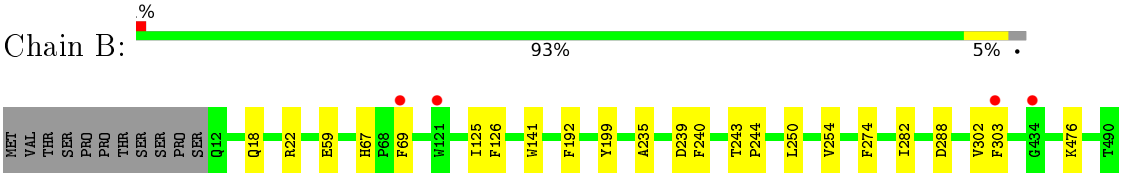
- Molecule 1: Apocarotenoid-15,15'-oxygenase

Chain A:



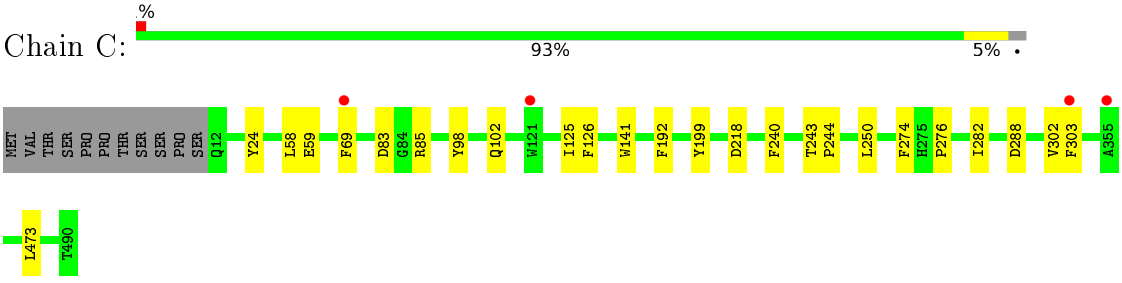
- Molecule 1: Apocarotenoid-15,15'-oxygenase

Chain B:



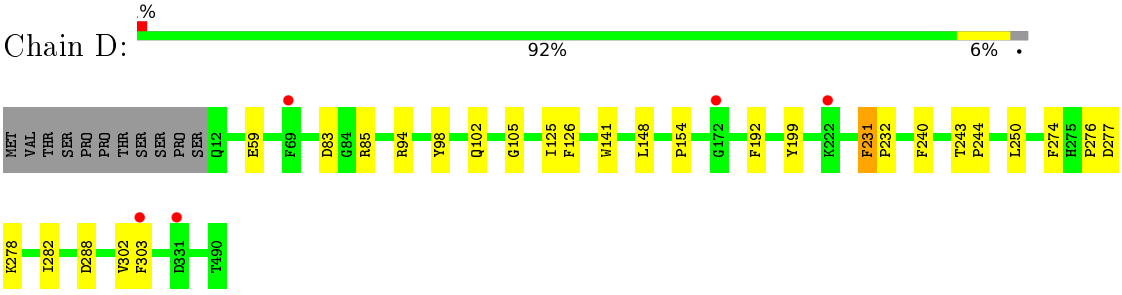
- Molecule 1: Apocarotenoid-15,15'-oxygenase

Chain C:



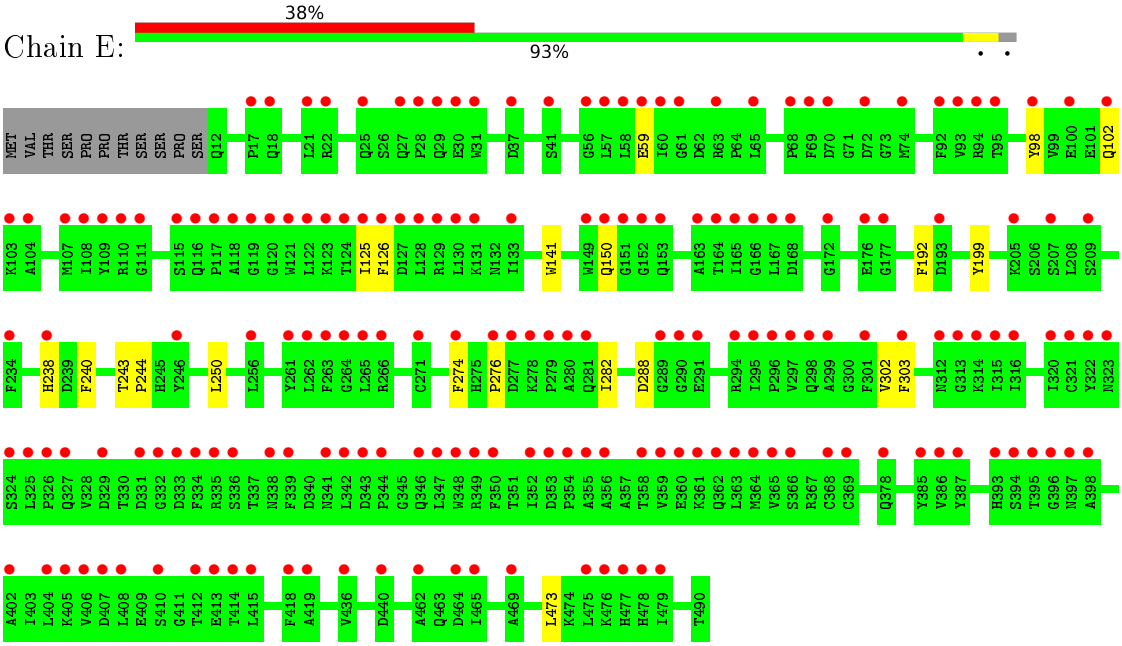
- Molecule 1: Apocarotenoid-15,15'-oxygenase

Chain D:



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

Chain E:


38%
93%
MET VAL THR SER PRO PRO THR SER SER PRO SER Q12 P17 Q18 L21 R22 Q25 S26 Q27 P28 Q29 E30 W31 D37 S41 G56 L57 L58 E59 I60 G61 D62 R63 P64 L65 P68 P69 D70 G71 D72 G73 M74 F92 V93 R94 T95 Y98 V99 E100 E101 Q102
K103 A104 M107 I108 Y109 R110 G111 S115 Q116 P117 A118 G119 G120 W121 L122 K123 T124 I125 F126 D127 L128 R129 L130 K131 N132 I133 W141 W149 Q150 G151 G152 Q153 A163 T164 I165 G166 L167 D168 G172 E176 G177 F192 D193 Y199 K205 S206 S207 L208 S209
F234 H238 D239 F240 T243 P244 H245 Y246 L250 L256 Y261 L262 F263 G264 L265 R266 C271 F274 H275 P276 D277 K278 P279 A280 Q281 I282 D288 G289 G290 E291 R294 I295 P296 V297 Q298 A299 G300 F301 V302 F303 N312 G313 K314 I315 I316 I320 G321 Y322 N323
S324 L325 P326 Q327 V328 D329 T330 D331 G332 D333 F334 R335 S336 T337 N338 F339 D340 N341 L342 D343 P344 G345 Q346 L347 W348 R349 F350 T351 I352 D353 P354 A355 A356 A357 T358 V359 E360 K361 Q362 L363 M364 V365 S366 R367 C368 C369 Q378 Y385 V386 Y387 H393 S394 T395 G396 N397 A398
A402 I403 L404 K405 V406 D407 L408 E409 S410 G411 T412 E413 T414 L415 F418 A419 V436 D440 A462 Q463 D464 I465 A469 L473 K474 L475 K476 H477 H478 I479 T490

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.53Å 125.50Å 203.60Å 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 2.77Å)	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 (4.94%)	DCC
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.*

[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

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

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:N	1:A:473:LEU:HD12	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:C:243:THR:HB	1:C:244:PRO:CD	2.47	0.44
1:B:18:GLN:HB3	1:D:102:GLN:OE1	2.17	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:N	1:E:473:LEU:HD12	2.35	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:B:22:ARG:NE	1:D:102:GLN:O	2.46	0.41
1:D:83:ASP:OD1	1:D:85:ARG:HB2	2.21	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:A:277:ASP:OD2	1:B:476:LYS:NZ	2.44	0.41
1:E:243:THR:HB	1:E:244:PRO:CD	2.50	0.41
1:C:218:ASP:C	1:C:218:ASP:OD1	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 (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	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

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%)	86	96
1	B	399/410 (97%)	396 (99%)	3 (1%)	86	96
1	C	399/410 (97%)	396 (99%)	3 (1%)	86	96
1	D	399/410 (97%)	394 (99%)	5 (1%)	76	93
1	E	399/410 (97%)	396 (99%)	3 (1%)	86	96
All	All	1995/2050 (97%)	1978 (99%)	17 (1%)	84	95

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

Some 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

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 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

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	479/490 (97%)	-0.34	5 (1%) 84 80	29, 49, 90, 141	0
1	B	479/490 (97%)	-0.25	4 (0%) 87 83	28, 49, 81, 132	0
1	C	479/490 (97%)	-0.24	4 (0%) 87 83	28, 52, 96, 125	0
1	D	479/490 (97%)	-0.19	5 (1%) 84 80	32, 57, 95, 128	0
1	E	479/490 (97%)	1.82	185 (38%) 0 0	80, 128, 171, 223	0
All	All	2395/2450 (97%)	0.16	203 (8%) 13 8	28, 57, 145, 223	0

All (203) 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	9.5
1	E	122	LEU	7.8
1	E	125	ILE	7.7
1	E	277	ASP	7.0
1	E	331	ASP	7.0
1	E	98	TYR	6.4
1	E	359	VAL	6.4
1	E	118	ALA	6.3
1	E	119	GLY	6.2
1	E	124	THR	6.2
1	E	281	GLN	6.2
1	E	274	PHE	6.2
1	E	126	PHE	6.0
1	E	348	TRP	5.9
1	E	279	PRO	5.7
1	E	296	PRO	5.5
1	E	462	ALA	5.2
1	E	130	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	333	ASP	5.0
1	E	476	LYS	4.9
1	E	344	PRO	4.9
1	E	265	LEU	4.9
1	E	264	GLY	4.7
1	E	341	ASN	4.7
1	E	18	GLN	4.4
1	E	355	ALA	4.4
1	E	298	GLN	4.4
1	E	334	PHE	4.4
1	E	61	GLY	4.4
1	E	396	GLY	4.4
1	E	60	ILE	4.4
1	E	299	ALA	4.4
1	E	58	LEU	4.3
1	E	350	PHE	4.3
1	E	261	TYR	4.3
1	E	342	LEU	4.2
1	E	338	ASN	4.2
1	E	276	PRO	4.1
1	E	128	LEU	4.1
1	E	356	ALA	4.1
1	E	94	ARG	4.1
1	E	266	ARG	4.1
1	E	393	HIS	4.0
1	E	343	ASP	4.0
1	E	256	LEU	4.0
1	E	436	VAL	4.0
1	E	332	GLY	3.9
1	E	93	VAL	3.9
1	E	323	ASN	3.9
1	C	303	PHE	3.9
1	E	418	PHE	3.9
1	E	397	ASN	3.8
1	E	163	ALA	3.8
1	E	312	ASN	3.8
1	E	289	GLY	3.7
1	E	131	LYS	3.7
1	E	405	LYS	3.7
1	E	100	GLU	3.7
1	E	415	LEU	3.7
1	E	297	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	354	PRO	3.6
1	E	21	LEU	3.6
1	E	398	ALA	3.6
1	E	315	ILE	3.5
1	E	295	ILE	3.5
1	E	313	GLY	3.5
1	E	413	GLU	3.5
1	E	294	ARG	3.5
1	E	262	LEU	3.5
1	E	404	LEU	3.5
1	E	123	LYS	3.4
1	E	362	GLN	3.4
1	E	464	ASP	3.4
1	E	325	LEU	3.4
1	E	465	ILE	3.4
1	E	56	GLY	3.4
1	E	69	PHE	3.4
1	E	419	ALA	3.4
1	E	395	THR	3.4
1	E	176	GLU	3.4
1	E	329	ASP	3.3
1	E	402	ALA	3.3
1	E	347	LEU	3.3
1	E	352	ILE	3.3
1	E	477	HIS	3.3
1	E	109	TYR	3.2
1	E	166	GLY	3.2
1	E	234	PHE	3.2
1	E	314	LYS	3.2
1	E	110	ARG	3.2
1	E	116	GLN	3.2
1	E	394	SER	3.2
1	E	238	HIS	3.1
1	E	167	LEU	3.1
1	E	368	CYS	3.1
1	E	475	LEU	3.1
1	E	102	GLN	3.1
1	E	207	SER	3.1
1	E	303	PHE	3.0
1	E	193	ASP	3.0
1	E	65	LEU	3.0
1	E	68	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	107	MET	3.0
1	A	69	PHE	3.0
1	E	339	PHE	3.0
1	E	129	ARG	3.0
1	E	414	THR	2.9
1	E	27	GLN	2.9
1	E	316	ILE	2.9
1	E	478	HIS	2.9
1	E	152	GLY	2.9
1	E	165	ILE	2.9
1	E	327	GLN	2.9
1	E	30	GLU	2.8
1	E	57	LEU	2.8
1	A	121	TRP	2.8
1	E	25	GLN	2.8
1	E	172	GLY	2.8
1	E	22	ARG	2.8
1	E	440	ASP	2.8
1	E	410	SER	2.8
1	E	149	TRP	2.8
1	E	17	PRO	2.7
1	E	291	GLU	2.7
1	E	153	GLN	2.7
1	B	69	PHE	2.7
1	E	385	TYR	2.7
1	E	127	ASP	2.7
1	E	349	ARG	2.7
1	E	346	GLN	2.7
1	E	407	ASP	2.6
1	E	301	PHE	2.6
1	E	104	ALA	2.6
1	E	205	LYS	2.6
1	E	364	MET	2.6
1	E	95	THR	2.6
1	C	69	PHE	2.6
1	E	92	PHE	2.6
1	E	324	SER	2.6
1	E	336	SER	2.6
1	E	360	GLU	2.5
1	E	335	ARG	2.5
1	E	59	GLU	2.5
1	E	74	MET	2.5

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

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Mol	Chain	Res	Type	RSRZ
1	E	366	SER	2.1
1	C	121	TRP	2.1
1	E	31	TRP	2.1
1	E	353	ASP	2.1
1	C	355	ALA	2.1
1	E	37	ASP	2.1
1	E	72	ASP	2.1
1	E	280	ALA	2.0
1	E	177	GLY	2.0
1	E	246	TYR	2.0
1	B	434	GLY	2.0
1	E	70	ASP	2.0
1	E	387	TYR	2.0
1	D	172	GLY	2.0
1	E	271	CYS	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^{th} 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(Å^2)	Q<0.9
2	FE2	E	501	1/1	0.40	0.33	0.64	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	0.93	0.10	-	75,75,75,75	0
2	FE2	D	501	1/1	0.98	0.14	-	74,74,74,74	0
2	FE2	A	501	1/1	0.96	0.08	-	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.