Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2016 – 04:42 PM EDT

PDB ID	:	5KJB
Title	:	Synechocystis apocarotenoid oxygenase (ACO) mutant - Glu150Asp
Authors	:	Sui, X.; Kiser, P.D.; Palczewski, K.
Deposited on	:	2016-06-18
Resolution	:	2.81 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:

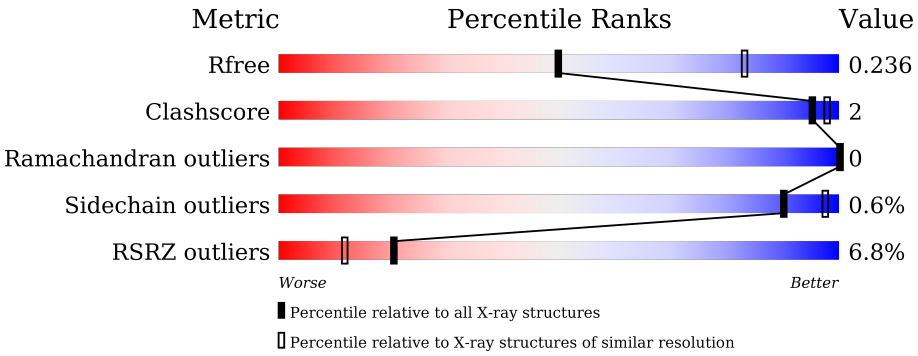
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.81 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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 >=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	94%
1	B	490	94%
1	C	490	93%
1	D	490	93% 5%
1	E	490	32% 94%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18909 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
			3767	2416	650	691	10			
1	B	479	Total	C	N	O	S	0	0	0
			3767	2416	650	691	10			
1	C	479	Total	C	N	O	S	0	0	0
			3767	2416	650	691	10			
1	D	479	Total	C	N	O	S	0	0	0
			3767	2416	650	691	10			
1	E	479	Total	C	N	O	S	0	0	0
			3767	2416	650	691	10			

There are 5 discrepancies between the modelled and reference sequences:

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

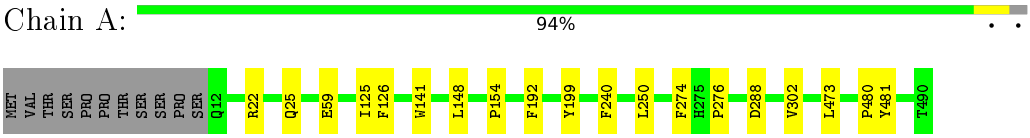
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	16	Total O 16 16	0	0
3	B	21	Total O 21 21	0	0
3	C	18	Total O 18 18	0	0
3	D	12	Total O 12 12	0	0
3	E	2	Total O 2 2	0	0

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.

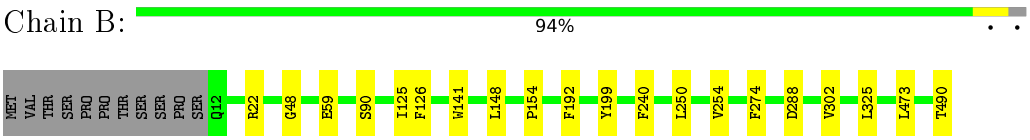
- Molecule 1: Apocarotenoid-15,15'-oxygenase

Chain A:



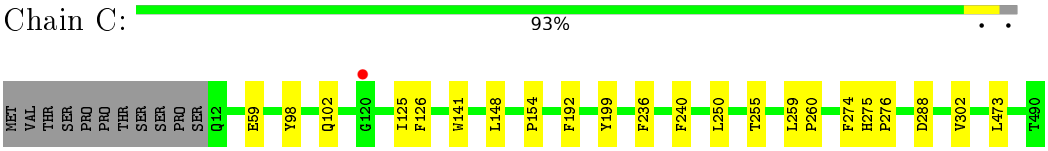
- Molecule 1: Apocarotenoid-15,15'-oxygenase

Chain B:



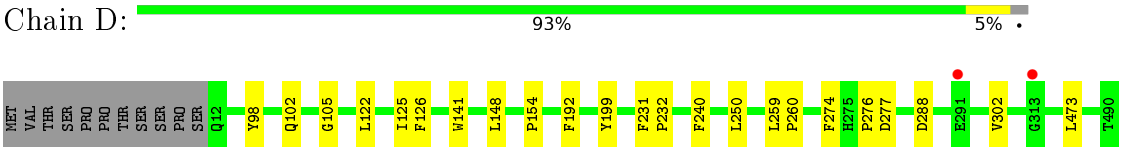
- Molecule 1: Apocarotenoid-15,15'-oxygenase

Chain C:



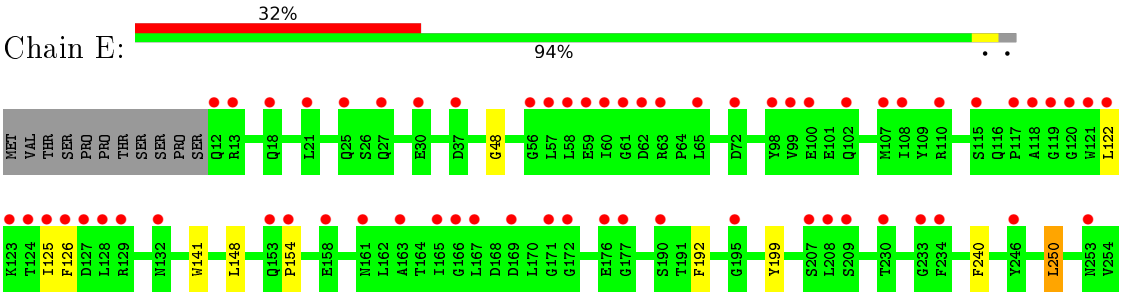
- Molecule 1: Apocarotenoid-15,15'-oxygenase

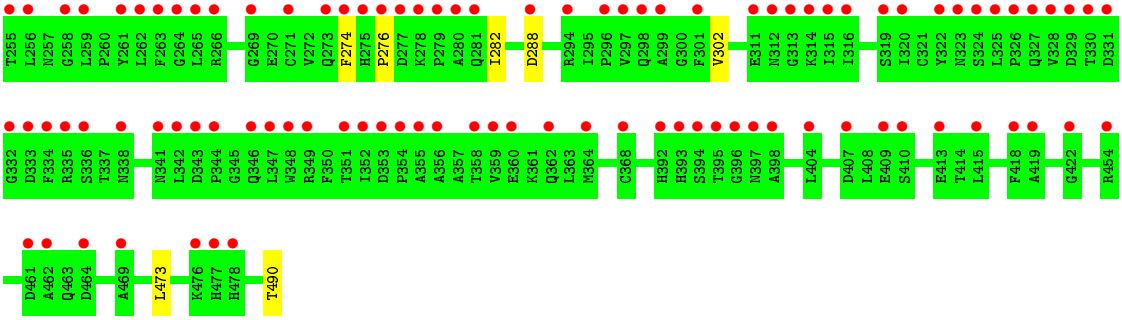
Chain D:



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

Chain E:




T255 L256 N257 G258 L259 P260 Y261 L262 F263 G264 L265 R266 G269 E270 C271 V272 Q273 F274 H275 P276 D277 K278 P279 A280 Q281 I282 D288 R294 I295 P296 V297 Q298 A299 G300 F301 V302 E311 N312 G313 K314 I315 I316 S319 I320 C321 Y322 N323 S324 L325 P326 Q327 V328 D329 T330 D331
G332 D333 F334 R335 S336 T337 N338 N341 L342 D343 P344 G345 Q346 L347 W348 R349 F350 T351 I352 D353 P354 A355 A356 A357 T358 V359 E360 K361 Q362 L363 M364 C368 H392 H393 S394 T395 G396 N397 A398 L404 D407 L408 E409 S410 E413 T414 L415 F418 A419 G422 R454
D461 A462 Q463 D464 A469 L473 K476 H477 H478 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	118.42Å 124.95Å 203.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.81 47.38 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.58-2.81) 99.9 (47.38-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.202 , 0.233 0.207 , 0.236	Depositor DCC
R_{free} test set	3573 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	62.5	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.5	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	0.94	EDS
Total number of atoms	18909	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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	0.57	0/3880	0.69	0/5284
1	B	0.58	0/3880	0.70	0/5284
1	C	0.55	0/3880	0.68	0/5284
1	D	0.54	0/3880	0.70	1/5284 (0.0%)
1	E	0.45	0/3880	0.66	2/5284 (0.0%)
All	All	0.54	0/19400	0.69	3/26420 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	277	ASP	CB-CG-OD1	6.51	124.16	118.30
1	E	250	LEU	CA-CB-CG	-6.20	101.04	115.30
1	E	250	LEU	CB-CG-CD2	5.86	120.96	111.00

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	3767	0	3657	10	0
1	B	3767	0	3657	13	0
1	C	3767	0	3657	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3767	0	3657	14	0
1	E	3767	0	3657	13	0
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	16	0	0	0	0
3	B	21	0	0	1	0
3	C	18	0	0	0	0
3	D	12	0	0	0	0
3	E	2	0	0	0	0
All	All	18909	0	18285	61	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 (61) 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:274:PHE:CZ	1:A:276:PRO:HA	2.18	0.79
1:C:274:PHE:CZ	1:C:276:PRO:HA	2.24	0.72
1:E:274:PHE:CZ	1:E:276:PRO:HA	2.25	0.71
1:D:274:PHE:CZ	1:D:276:PRO:HA	2.29	0.67
1:E:250:LEU:CD1	1:E:282:ILE:HG12	2.29	0.63
1:A:250:LEU:HD22	1:A:302:VAL:HB	1.85	0.59
1:D:250:LEU:HD22	1:D:302:VAL:HB	1.85	0.58
1:B:250:LEU:HD22	1:B:302:VAL:HB	1.85	0.58
1:C:250:LEU:HD22	1:C:302:VAL:HB	1.85	0.58
1:B:90:SER:OG	3:B:601:HOH:O	2.18	0.56
1:B:125:ILE:HG12	1:B:126:PHE:CD2	2.45	0.52
1:E:125:ILE:HG12	1:E:126:PHE:CD2	2.46	0.51
1:E:250:LEU:HD22	1:E:302:VAL:HG21	1.93	0.51
1:D:192:PHE:CE1	1:D:288:ASP:HB3	2.46	0.51
1:D:231:PHE:CD1	1:D:232:PRO:HD2	2.46	0.51
1:C:125:ILE:HG12	1:C:126:PHE:CD2	2.45	0.50
1:B:192:PHE:CE1	1:B:288:ASP:HB3	2.47	0.50
1:D:231:PHE:CE2	1:D:232:PRO:O	2.64	0.50
1:A:125:ILE:HG12	1:A:126:PHE:CD2	2.46	0.50
1:D:125:ILE:HG12	1:D:126:PHE:CD2	2.46	0.49
1:E:148:LEU:HD23	1:E:154:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:PHE:CE1	1:C:288:ASP:HB3	2.48	0.49
1:A:192:PHE:CE1	1:A:288:ASP:HB3	2.47	0.49
1:C:255:THR:HG23	1:C:275:HIS:HE1	1.78	0.49
1:E:192:PHE:CE1	1:E:288:ASP:HB3	2.49	0.48
1:D:148:LEU:HD23	1:D:154:PRO:HB3	1.95	0.48
1:E:250:LEU:HD12	1:E:282:ILE:HG12	1.96	0.47
1:A:22:ARG:HG3	1:A:25:GLN:HE21	1.79	0.47
1:C:148:LEU:HD23	1:C:154:PRO:HB3	1.96	0.47
1:A:141:TRP:CE2	1:A:199:TYR:HB2	2.50	0.46
1:A:148:LEU:HD23	1:A:154:PRO:HB3	1.97	0.46
1:B:141:TRP:CE2	1:B:199:TYR:HB2	2.50	0.46
1:C:473:LEU:CD1	1:C:473:LEU:N	2.79	0.46
1:D:250:LEU:HD23	1:D:250:LEU:C	2.36	0.46
1:B:148:LEU:HD23	1:B:154:PRO:HB3	1.96	0.45
1:E:141:TRP:CE2	1:E:199:TYR:HB2	2.51	0.45
1:C:473:LEU:HD12	1:C:473:LEU:N	2.31	0.45
1:D:141:TRP:CE2	1:D:199:TYR:HB2	2.51	0.44
1:C:255:THR:HG23	1:C:275:HIS:CE1	2.53	0.44
1:B:473:LEU:CD1	1:B:473:LEU:N	2.81	0.43
1:C:141:TRP:CE2	1:C:199:TYR:HB2	2.53	0.43
1:A:473:LEU:N	1:A:473:LEU:CD1	2.81	0.43
1:B:274:PHE:CG	1:B:325:LEU:HD12	2.53	0.43
1:C:98:TYR:O	1:C:102:GLN:HG2	2.18	0.43
1:E:250:LEU:HD22	1:E:302:VAL:CG2	2.47	0.43
1:B:473:LEU:HD12	1:B:473:LEU:N	2.33	0.43
1:D:473:LEU:N	1:D:473:LEU:CD1	2.82	0.43
1:D:473:LEU:N	1:D:473:LEU:HD12	2.34	0.43
1:B:22:ARG:NH2	1:D:105:GLY:HA2	2.34	0.43
1:A:473:LEU:N	1:A:473:LEU:HD12	2.34	0.42
1:B:250:LEU:HD23	1:B:250:LEU:C	2.40	0.42
1:B:254:VAL:HG12	1:B:274:PHE:CD1	2.55	0.42
1:E:250:LEU:HD22	1:E:302:VAL:HB	2.01	0.42
1:E:473:LEU:HD12	1:E:473:LEU:N	2.34	0.41
1:C:259:LEU:N	1:C:260:PRO:CD	2.83	0.41
1:E:473:LEU:CD1	1:E:473:LEU:N	2.83	0.41
1:B:48:GLY:HA2	1:B:490:THR:HG23	2.02	0.41
1:D:98:TYR:O	1:D:102:GLN:HG2	2.21	0.41
1:D:259:LEU:N	1:D:260:PRO:CD	2.83	0.41
1:A:480:PRO:O	1:A:481:TYR:C	2.58	0.41
1:E:48:GLY:HA2	1:E:490:THR:HG23	2.03	0.41

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%)	461 (97%)	16 (3%)	0	100	100
1	C	477/490 (97%)	462 (97%)	15 (3%)	0	100	100
1	D	477/490 (97%)	460 (96%)	17 (4%)	0	100	100
1	E	477/490 (97%)	463 (97%)	14 (3%)	0	100	100
All	All	2385/2450 (97%)	2307 (97%)	78 (3%)	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%)	397 (100%)	2 (0%)	92	98
1	B	399/410 (97%)	397 (100%)	2 (0%)	92	98
1	C	399/410 (97%)	396 (99%)	3 (1%)	86	97
1	D	399/410 (97%)	397 (100%)	2 (0%)	92	98
1	E	399/410 (97%)	397 (100%)	2 (0%)	92	98
All	All	1995/2050 (97%)	1984 (99%)	11 (1%)	90	97

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	240	PHE
1	B	59	GLU
1	B	240	PHE
1	C	59	GLU
1	C	236	PHE
1	C	240	PHE
1	D	122	LEU
1	D	240	PHE
1	E	122	LEU
1	E	240	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	275	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 carbohydrates 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

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%)	-0.32	0 100 100	29, 54, 92, 128	0
1	B	479/490 (97%)	-0.32	0 100 100	27, 51, 84, 131	0
1	C	479/490 (97%)	-0.30	1 (0%) 95 94	30, 56, 95, 148	0
1	D	479/490 (97%)	-0.18	2 (0%) 93 90	30, 60, 107, 135	0
1	E	479/490 (97%)	1.61	159 (33%) 0 0	78, 131, 174, 227	0
All	All	2395/2450 (97%)	0.10	162 (6%) 20 12	27, 61, 148, 227	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	333	ASP	8.6
1	E	119	GLY	7.6
1	E	263	PHE	7.2
1	E	122	LEU	7.1
1	E	124	THR	6.6
1	E	296	PRO	6.6
1	E	332	GLY	6.5
1	E	277	ASP	6.1
1	E	334	PHE	5.8
1	E	117	PRO	5.8
1	E	62	ASP	5.8
1	E	344	PRO	5.8
1	E	331	ASP	5.6
1	E	166	GLY	5.5
1	E	359	VAL	5.4
1	E	118	ALA	5.2
1	E	120	GLY	5.1
1	E	338	ASN	4.9
1	E	61	GLY	4.9
1	E	125	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	274	PHE	4.7
1	E	279	PRO	4.6
1	E	126	PHE	4.5
1	E	171	GLY	4.5
1	E	59	GLU	4.4
1	E	298	GLN	4.3
1	E	266	ARG	4.3
1	E	313	GLY	4.2
1	E	195	GLY	4.1
1	E	348	TRP	4.1
1	E	121	TRP	4.1
1	E	299	ALA	4.0
1	E	100	GLU	4.0
1	E	330	THR	3.9
1	E	12	GLN	3.9
1	E	123	LYS	3.9
1	E	336	SER	3.9
1	E	264	GLY	3.9
1	E	169	ASP	3.8
1	E	256	LEU	3.8
1	E	271	CYS	3.8
1	E	464	ASP	3.8
1	E	394	SER	3.8
1	E	63	ARG	3.7
1	E	312	ASN	3.7
1	E	314	LYS	3.7
1	E	262	LEU	3.6
1	E	396	GLY	3.6
1	E	343	ASP	3.6
1	E	398	ALA	3.6
1	E	176	GLU	3.6
1	E	57	LEU	3.5
1	E	404	LEU	3.5
1	E	327	GLN	3.5
1	E	341	ASN	3.5
1	E	107	MET	3.5
1	E	419	ALA	3.5
1	E	476	LYS	3.5
1	E	364	MET	3.5
1	E	351	THR	3.4
1	E	280	ALA	3.4
1	E	322	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	410	SER	3.4
1	E	58	LEU	3.4
1	E	294	ARG	3.3
1	E	265	LEU	3.3
1	E	397	ASN	3.3
1	E	281	GLN	3.3
1	E	395	THR	3.3
1	E	418	PHE	3.3
1	E	368	CYS	3.3
1	E	356	ALA	3.2
1	E	72	ASP	3.2
1	E	288	ASP	3.2
1	E	358	THR	3.2
1	E	324	SER	3.2
1	E	18	GLN	3.1
1	E	360	GLU	3.1
1	E	276	PRO	3.1
1	E	207	SER	3.0
1	E	319	SER	3.0
1	E	27	GLN	3.0
1	E	25	GLN	2.9
1	E	316	ILE	2.9
1	E	335	ARG	2.9
1	E	462	ALA	2.9
1	E	311	GLU	2.9
1	E	362	GLN	2.9
1	E	102	GLN	2.8
1	E	108	ILE	2.8
1	E	297	VAL	2.8
1	E	392	HIS	2.8
1	E	354	PRO	2.8
1	E	301	PHE	2.8
1	E	234	PHE	2.8
1	E	355	ALA	2.8
1	E	353	ASP	2.8
1	E	454	ARG	2.8
1	E	163	ALA	2.7
1	E	352	ILE	2.7
1	E	65	LEU	2.7
1	E	128	LEU	2.7
1	E	393	HIS	2.7
1	E	261	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	165	ILE	2.7
1	E	209	SER	2.7
1	E	320	ILE	2.7
1	E	167	LEU	2.7
1	E	259	LEU	2.6
1	E	60	ILE	2.6
1	E	478	HIS	2.6
1	E	253	ASN	2.6
1	E	342	LEU	2.6
1	E	255	THR	2.6
1	E	315	ILE	2.6
1	E	329	ASP	2.6
1	E	110	ARG	2.6
1	E	172	GLY	2.5
1	E	190	SER	2.5
1	E	275	HIS	2.5
1	E	246	TYR	2.5
1	E	349	ARG	2.4
1	C	120	GLY	2.4
1	E	208	LEU	2.4
1	E	98	TYR	2.4
1	E	56	GLY	2.4
1	E	409	GLU	2.3
1	E	37	ASP	2.3
1	E	407	ASP	2.3
1	E	323	ASN	2.3
1	E	258	GLY	2.3
1	E	469	ALA	2.3
1	E	278	LYS	2.3
1	E	129	ARG	2.3
1	E	413	GLU	2.3
1	E	13	ARG	2.3
1	E	21	LEU	2.3
1	D	313	GLY	2.2
1	E	115	SER	2.2
1	E	153	GLN	2.2
1	E	273	GLN	2.2
1	E	177	GLY	2.2
1	E	132	ASN	2.2
1	E	230	THR	2.2
1	E	415	LEU	2.2
1	E	158	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	347	LEU	2.1
1	E	99	VAL	2.1
1	E	461	ASP	2.1
1	E	346	GLN	2.1
1	E	233	GLY	2.1
1	E	326	PRO	2.1
1	D	291	GLU	2.1
1	E	328	VAL	2.1
1	E	161	ASN	2.1
1	E	325	LEU	2.0
1	E	30	GLU	2.0
1	E	127	ASP	2.0
1	E	477	HIS	2.0
1	E	269	GLY	2.0
1	E	422	GLY	2.0
1	E	154	PRO	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	0.53	0.21	0.19	147,147,147,147	0
2	FE2	C	501	1/1	0.86	0.18	-0.39	89,89,89,89	0
2	FE2	D	501	1/1	0.80	0.16	-	87,87,87,87	0
2	FE2	B	501	1/1	0.86	0.14	-	86,86,86,86	0
2	FE2	A	501	1/1	0.92	0.11	-	85,85,85,85	0

6.5 Other polymers (i)

There are no such residues in this entry.