



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:29 am BST

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

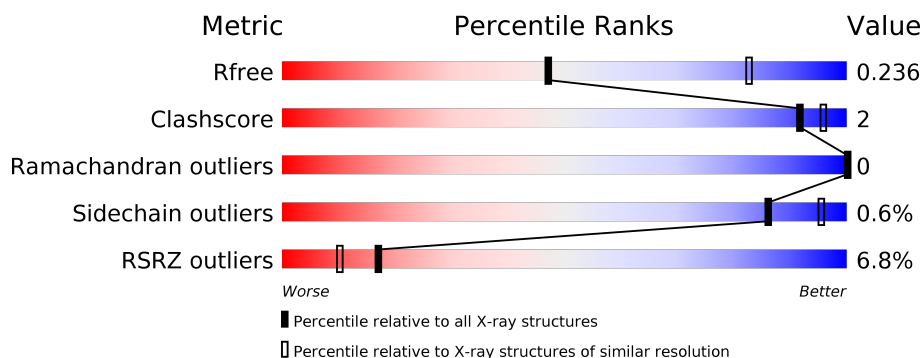
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (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 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 $\leq 5\%$. 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 style="width: 94%;"></div> <div>94%</div> </div>
1	B	490	<div> <div style="width: 94%;"></div> <div>94%</div> </div>
1	C	490	<div> <div style="width: 93%;"></div> <div>93%</div> </div>
1	D	490	<div> <div style="width: 93%;"></div> <div>93%</div> </div>
1	E	490	<div> <div style="width: 32%; background-color: red;"></div> <div>32%</div> <div style="width: 94%;"></div> <div>94%</div> </div>

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 16	O 16	0	0
3	B	21	Total 21	O 21	0	0
3	C	18	Total 18	O 18	0	0
3	D	12	Total 12	O 12	0	0
3	E	2	Total 2	O 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 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

Chain A: 



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

Chain B: 



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

Chain C: 



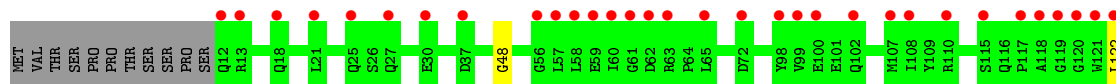
- Molecule 1: Apocarotenoid-15,15'-oxygenase

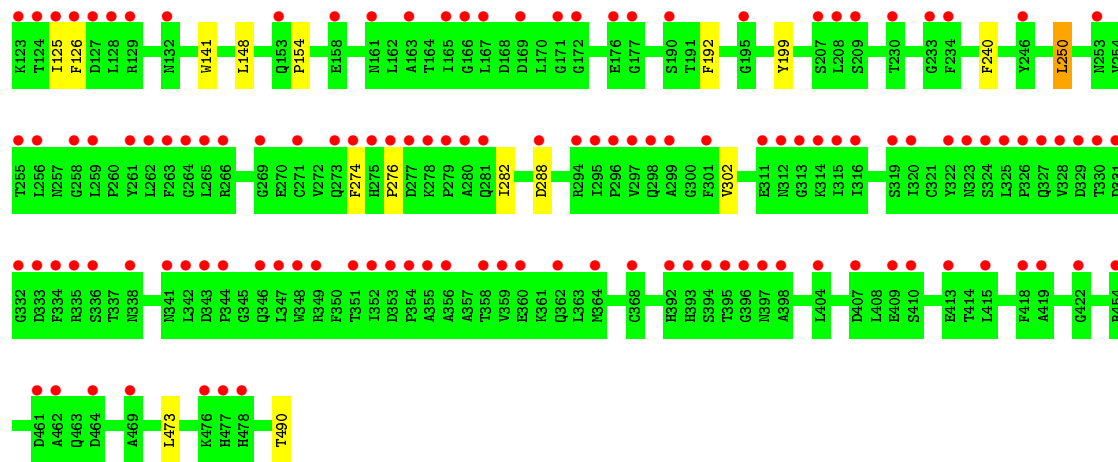
Chain D: 



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

Chain E: 





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	3583 reflections (4.80%)	wwPDB-VP
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	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [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	0.57	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(°)	Ideal(°)
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 [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	3767	0	3657	10	0
1	B	3767	0	3657	13	0
1	C	3767	0	3657	12	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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%)	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

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%)	88	96
1	B	399/410 (97%)	397 (100%)	2 (0%)	88	96
1	C	399/410 (97%)	396 (99%)	3 (1%)	81	94
1	D	399/410 (97%)	397 (100%)	2 (0%)	88	96
1	E	399/410 (97%)	397 (100%)	2 (0%)	88	96
All	All	1995/2050 (97%)	1984 (99%)	11 (1%)	86	95

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, 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%)	-0.32	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%)	92	91	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%)	17	10	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	7.7
1	E	122	LEU	7.2
1	E	263	PHE	7.1
1	E	332	GLY	6.6
1	E	296	PRO	6.6
1	E	124	THR	6.5
1	E	277	ASP	6.1
1	E	334	PHE	5.9
1	E	62	ASP	5.8
1	E	344	PRO	5.8
1	E	117	PRO	5.7
1	E	331	ASP	5.6
1	E	359	VAL	5.5
1	E	166	GLY	5.4
1	E	118	ALA	5.2
1	E	120	GLY	5.2
1	E	61	GLY	5.2
1	E	338	ASN	5.0
1	E	125	ILE	4.8

Continued on next page...

Continued from previous page...

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	59	GLU	4.5
1	E	171	GLY	4.5
1	E	298	GLN	4.3
1	E	266	ARG	4.3
1	E	313	GLY	4.1
1	E	195	GLY	4.1
1	E	348	TRP	4.1
1	E	121	TRP	4.0
1	E	100	GLU	4.0
1	E	264	GLY	4.0
1	E	299	ALA	4.0
1	E	330	THR	4.0
1	E	336	SER	3.9
1	E	271	CYS	3.9
1	E	12	GLN	3.9
1	E	123	LYS	3.8
1	E	394	SER	3.8
1	E	256	LEU	3.8
1	E	169	ASP	3.8
1	E	464	ASP	3.8
1	E	314	LYS	3.7
1	E	63	ARG	3.7
1	E	312	ASN	3.7
1	E	404	LEU	3.7
1	E	262	LEU	3.6
1	E	176	GLU	3.6
1	E	57	LEU	3.6
1	E	343	ASP	3.6
1	E	398	ALA	3.6
1	E	396	GLY	3.6
1	E	341	ASN	3.5
1	E	364	MET	3.5
1	E	476	LYS	3.5
1	E	107	MET	3.5
1	E	327	GLN	3.5
1	E	419	ALA	3.4
1	E	58	LEU	3.4
1	E	322	TYR	3.4
1	E	351	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	397	ASN	3.4
1	E	294	ARG	3.3
1	E	280	ALA	3.3
1	E	410	SER	3.3
1	E	265	LEU	3.3
1	E	395	THR	3.3
1	E	418	PHE	3.3
1	E	368	CYS	3.3
1	E	281	GLN	3.3
1	E	358	THR	3.2
1	E	324	SER	3.2
1	E	72	ASP	3.2
1	E	288	ASP	3.2
1	E	356	ALA	3.1
1	E	18	GLN	3.1
1	E	360	GLU	3.1
1	E	207	SER	3.1
1	E	276	PRO	3.1
1	E	27	GLN	3.0
1	E	319	SER	3.0
1	E	335	ARG	3.0
1	E	25	GLN	2.9
1	E	462	ALA	2.9
1	E	316	ILE	2.9
1	E	311	GLU	2.9
1	E	362	GLN	2.9
1	E	108	ILE	2.9
1	E	297	VAL	2.9
1	E	102	GLN	2.8
1	E	354	PRO	2.8
1	E	392	HIS	2.8
1	E	128	LEU	2.8
1	E	301	PHE	2.8
1	E	163	ALA	2.8
1	E	454	ARG	2.7
1	E	355	ALA	2.7
1	E	352	ILE	2.7
1	E	353	ASP	2.7
1	E	234	PHE	2.7
1	E	261	TYR	2.7
1	E	65	LEU	2.7
1	E	165	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	315	ILE	2.7
1	E	393	HIS	2.7
1	E	209	SER	2.6
1	E	320	ILE	2.6
1	E	167	LEU	2.6
1	E	329	ASP	2.6
1	E	255	THR	2.6
1	E	478	HIS	2.6
1	E	259	LEU	2.6
1	E	253	ASN	2.6
1	E	342	LEU	2.6
1	E	60	ILE	2.5
1	E	172	GLY	2.5
1	E	110	ARG	2.5
1	E	275	HIS	2.5
1	E	246	TYR	2.5
1	E	208	LEU	2.5
1	E	98	TYR	2.4
1	E	190	SER	2.4
1	C	120	GLY	2.4
1	E	349	ARG	2.4
1	E	407	ASP	2.4
1	E	409	GLU	2.3
1	E	37	ASP	2.3
1	E	56	GLY	2.3
1	E	278	LYS	2.3
1	E	469	ALA	2.3
1	E	115	SER	2.3
1	E	323	ASN	2.3
1	E	413	GLU	2.3
1	E	129	ARG	2.3
1	D	313	GLY	2.3
1	E	258	GLY	2.3
1	E	13	ARG	2.3
1	E	21	LEU	2.2
1	E	153	GLN	2.2
1	E	230	THR	2.2
1	E	273	GLN	2.2
1	E	177	GLY	2.2
1	E	233	GLY	2.2
1	E	158	GLU	2.1
1	E	99	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	328	VAL	2.1
1	E	347	LEU	2.1
1	E	415	LEU	2.1
1	E	132	ASN	2.1
1	E	325	LEU	2.1
1	E	346	GLN	2.1
1	E	461	ASP	2.1
1	D	291	GLU	2.1
1	E	269	GLY	2.1
1	E	477	HIS	2.1
1	E	422	GLY	2.1
1	E	30	GLU	2.1
1	E	161	ASN	2.1
1	E	326	PRO	2.0
1	E	127	ASP	2.0
1	E	295	ILE	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. 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	0.53	0.21	147,147,147,147	0
2	FE2	D	501	1/1	0.80	0.16	87,87,87,87	0
2	FE2	C	501	1/1	0.86	0.18	89,89,89,89	0
2	FE2	B	501	1/1	0.86	0.14	86,86,86,86	0
2	FE2	A	501	1/1	0.93	0.11	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.