



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:56 am GMT

PDB ID : 3QHB  
Title : Crystal structure of oxidized Symerythrin from *Cyanophora paradoxa*  
Authors : Cooley, R.B.; Arp, D.J.; Karplus, P.A.  
Deposited on : 2011-01-25  
Resolution : 1.20 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	:	trunk28620
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)	:	recalc28949

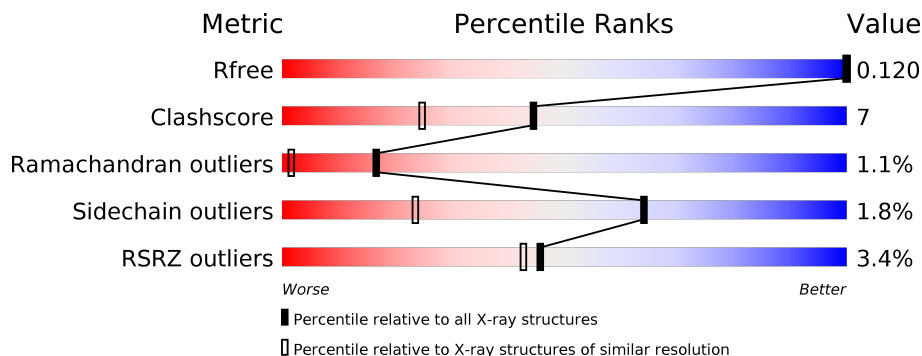
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.20 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	1131 (1.24-1.16)
Clashscore	112137	1201 (1.24-1.16)
Ramachandran outliers	110173	1148 (1.24-1.16)
Sidechain outliers	110143	1147 (1.24-1.16)
RSRZ outliers	101464	1132 (1.24-1.16)

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	179	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>5%</div> </div> </div>
1	B	179	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3534 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 Symerythrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	17	0
			1491	934	246	301	10			
1	B	179	Total	C	N	O	S	0	17	0
			1484	930	244	300	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Fe	0	0
			2	2		
2	A	2	Total	Fe	0	0
			2	2		

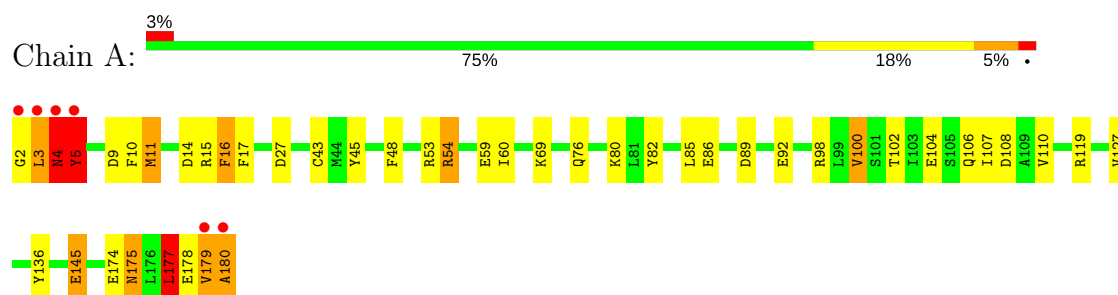
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	270	Total	O	0	0
			270	270		
3	B	285	Total	O	0	0
			285	285		

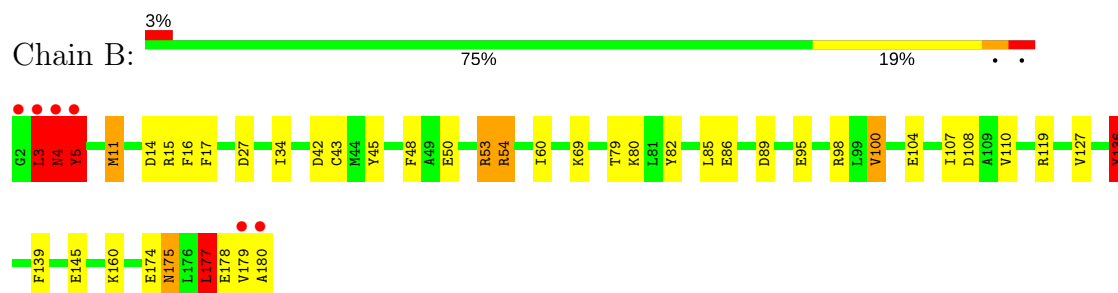
### 3 Residue-property plots [i](#)

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: Symerythrin



#### • Molecule 1: Symerythrin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.59Å 81.59Å 46.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.60 – 1.20 30.60 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.60-1.20) 99.9 (30.60-1.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.45 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.101 , 0.125 0.099 , 0.120	Depositor DCC
$R_{free}$ test set	5397 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	9.1	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.487 for -h,-k,l 0.025 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	3534	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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: FE

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	0.96	2/1543 (0.1%)	2.02	71/2083 (3.4%)
1	B	0.94	0/1539	1.98	64/2079 (3.1%)
All	All	0.95	2/3082 (0.1%)	2.00	135/4162 (3.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	GLN	CD-NE2	-5.68	1.18	1.32
1	A	69	LYS	CE-NZ	5.22	1.62	1.49

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	ARG	NE-CZ-NH1	-20.62	109.99	120.30
1	A	108	ASP	CB-CG-OD2	-18.59	101.57	118.30
1	B	54	ARG	NE-CZ-NH2	17.33	128.96	120.30
1	A	54	ARG	NE-CZ-NH1	17.27	128.93	120.30
1	A	11[A]	MET	CG-SD-CE	-16.18	74.31	100.20
1	A	11[B]	MET	CG-SD-CE	-16.18	74.31	100.20
1	A	108	ASP	CB-CG-OD1	14.89	131.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	ARG	CD-NE-CZ	14.37	143.71	123.60
1	A	104	GLU	OE1-CD-OE2	13.24	139.19	123.30
1	A	179	VAL	CG1-CB-CG2	12.52	130.93	110.90
1	A	3	LEU	CB-CG-CD2	11.59	130.71	111.00
1	B	3	LEU	CB-CG-CD2	11.51	130.57	111.00
1	B	98	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	B	54	ARG	NE-CZ-NH1	-11.35	114.63	120.30
1	B	108	ASP	CB-CG-OD2	-11.30	108.13	118.30
1	B	179	VAL	CG1-CB-CG2	11.08	128.62	110.90
1	A	180	ALA	CA-C-O	-11.07	96.86	120.10
1	B	14	ASP	CB-CG-OD2	10.71	127.94	118.30
1	A	136[A]	TYR	CB-CG-CD1	10.69	127.41	121.00
1	A	136[B]	TYR	CB-CG-CD1	10.69	127.41	121.00
1	A	27	ASP	CB-CG-OD2	10.49	127.74	118.30
1	B	177	LEU	O-C-N	-10.39	106.07	122.70
1	A	98	ARG	NE-CZ-NH2	10.29	125.44	120.30
1	B	15	ARG	NE-CZ-NH2	10.22	125.41	120.30
1	A	14	ASP	CB-CG-OD2	10.04	127.34	118.30
1	B	180	ALA	CA-C-O	-9.89	99.33	120.10
1	B	42[A]	ASP	CB-CG-OD1	9.75	127.07	118.30
1	B	42[B]	ASP	CB-CG-OD1	9.75	127.07	118.30
1	A	82	TYR	CG-CD2-CE2	-9.73	113.52	121.30
1	A	100	VAL	CA-CB-CG1	-9.51	96.63	110.90
1	B	104	GLU	OE1-CD-OE2	9.43	134.61	123.30
1	A	177	LEU	O-C-N	-9.33	107.77	122.70
1	A	54	ARG	NE-CZ-NH2	-9.15	115.73	120.30
1	B	5[A]	TYR	CD1-CE1-CZ	9.09	127.98	119.80
1	B	5[B]	TYR	CD1-CE1-CZ	9.09	127.98	119.80
1	A	5[A]	TYR	CD1-CE1-CZ	8.97	127.87	119.80
1	A	5[B]	TYR	CD1-CE1-CZ	8.97	127.87	119.80
1	B	179	VAL	CB-CA-C	8.86	128.24	111.40
1	A	98	ARG	NE-CZ-NH1	-8.81	115.90	120.30
1	B	50	GLU	OE1-CD-OE2	8.78	133.83	123.30
1	A	80	LYS	CD-CE-NZ	8.75	131.83	111.70
1	A	54	ARG	CD-NE-CZ	8.69	135.77	123.60
1	B	86	GLU	CG-CD-OE2	-8.66	100.99	118.30
1	B	136[A]	TYR	CB-CG-CD1	8.30	125.98	121.00
1	B	136[B]	TYR	CB-CG-CD1	8.30	125.98	121.00
1	A	69	LYS	CD-CE-NZ	-8.28	92.66	111.70
1	B	53[A]	ARG	NE-CZ-NH1	-8.23	116.18	120.30
1	B	53[B]	ARG	NE-CZ-NH1	-8.23	116.18	120.30
1	A	85	LEU	CB-CG-CD2	8.20	124.94	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	TYR	CB-CG-CD2	-8.09	116.14	121.00
1	B	80	LYS	CD-CE-NZ	8.08	130.28	111.70
1	B	45	TYR	CB-CG-CD2	7.77	125.66	121.00
1	A	45	TYR	CB-CG-CD2	7.69	125.61	121.00
1	B	86	GLU	CG-CD-OE1	7.67	133.65	118.30
1	B	100	VAL	CA-CB-CG1	-7.63	99.45	110.90
1	B	175[A]	ASN	CB-CG-OD1	7.63	136.86	121.60
1	B	175[B]	ASN	CB-CG-OD1	7.63	136.86	121.60
1	B	82	TYR	CG-CD2-CE2	-7.61	115.21	121.30
1	B	5[A]	TYR	CZ-CE2-CD2	7.56	126.60	119.80
1	B	5[B]	TYR	CZ-CE2-CD2	7.56	126.60	119.80
1	A	100	VAL	CA-CB-CG2	7.52	122.17	110.90
1	B	85	LEU	CB-CG-CD2	7.40	123.58	111.00
1	B	145[A]	GLU	OE1-CD-OE2	-7.32	114.52	123.30
1	B	145[B]	GLU	OE1-CD-OE2	-7.32	114.52	123.30
1	B	179	VAL	CA-CB-CG2	7.31	121.87	110.90
1	A	178	GLU	O-C-N	-7.26	111.08	122.70
1	A	178	GLU	CB-CA-C	7.18	124.77	110.40
1	B	15	ARG	CD-NE-CZ	7.14	133.60	123.60
1	A	104	GLU	CG-CD-OE1	-7.10	104.10	118.30
1	A	86	GLU	CG-CD-OE2	-7.10	104.10	118.30
1	A	175[A]	ASN	CB-CG-OD1	7.05	135.70	121.60
1	A	175[B]	ASN	CB-CG-OD1	7.05	135.70	121.60
1	A	179	VAL	CB-CA-C	6.99	124.69	111.40
1	B	108	ASP	CB-CG-OD1	6.93	124.54	118.30
1	A	100	VAL	CB-CA-C	6.90	124.50	111.40
1	A	53[A]	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	53[B]	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	177	LEU	CB-CG-CD1	6.87	122.69	111.00
1	A	180	ALA	CB-CA-C	6.78	120.27	110.10
1	B	82	TYR	CB-CG-CD2	-6.78	116.93	121.00
1	A	89	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	B	178	GLU	O-C-N	-6.72	111.95	122.70
1	B	175[A]	ASN	CB-CG-ND2	-6.67	100.70	116.70
1	B	175[B]	ASN	CB-CG-ND2	-6.67	100.70	116.70
1	A	86	GLU	CA-CB-CG	6.50	127.70	113.40
1	B	5[A]	TYR	CE1-CZ-CE2	-6.36	109.62	119.80
1	B	5[B]	TYR	CE1-CZ-CE2	-6.36	109.62	119.80
1	B	100	VAL	CA-CB-CG2	6.36	120.43	110.90
1	B	69	LYS	CD-CE-NZ	-6.31	97.18	111.70
1	A	27	ASP	OD1-CG-OD2	-6.28	111.37	123.30
1	A	48	PHE	CB-CG-CD1	6.24	125.17	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	GLU	CG-CD-OE2	-6.16	105.97	118.30
1	A	119	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	A	16[A]	PHE	CB-CG-CD1	5.92	124.94	120.80
1	A	16[B]	PHE	CB-CG-CD1	5.92	124.94	120.80
1	A	145[A]	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	A	145[B]	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	B	180	ALA	N-CA-CB	5.87	118.31	110.10
1	A	59	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	A	177	LEU	CB-CG-CD1	5.74	120.76	111.00
1	A	5[A]	TYR	CE1-CZ-CE2	-5.72	110.64	119.80
1	A	5[B]	TYR	CE1-CZ-CE2	-5.72	110.64	119.80
1	B	119	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	54	ARG	CB-CG-CD	5.69	126.38	111.60
1	A	2	GLY	O-C-N	-5.66	113.64	122.70
1	B	11[A]	MET	CG-SD-CE	-5.64	91.17	100.20
1	B	11[B]	MET	CG-SD-CE	-5.64	91.17	100.20
1	B	98	ARG	NH1-CZ-NH2	-5.58	113.26	119.40
1	A	175[A]	ASN	CB-CG-ND2	-5.56	103.35	116.70
1	A	175[B]	ASN	CB-CG-ND2	-5.56	103.35	116.70
1	B	100	VAL	CB-CA-C	5.52	121.88	111.40
1	B	48	PHE	CB-CG-CD1	5.51	124.66	120.80
1	B	139	PHE	CB-CG-CD1	5.48	124.63	120.80
1	A	3	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	102[A]	THR	CA-CB-CG2	5.46	120.05	112.40
1	A	102[B]	THR	CA-CB-CG2	5.46	120.05	112.40
1	A	106	GLN	CB-CG-CD	-5.45	97.44	111.60
1	A	5[A]	TYR	CZ-CE2-CD2	5.45	124.70	119.80
1	A	5[B]	TYR	CZ-CE2-CD2	5.45	124.70	119.80
1	B	178	GLU	CB-CA-C	5.39	121.18	110.40
1	B	27	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	86	GLU	CA-CB-CG	5.36	125.20	113.40
1	A	2	GLY	CA-C-N	5.31	128.88	117.20
1	A	53[A]	ARG	CD-NE-CZ	5.27	130.97	123.60
1	A	53[B]	ARG	CD-NE-CZ	5.27	130.97	123.60
1	A	85	LEU	CB-CA-C	-5.20	100.32	110.20
1	A	15	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	136[A]	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	136[B]	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	86	GLU	CG-CD-OE1	5.10	128.50	118.30
1	B	42[A]	ASP	N-CA-CB	5.07	119.73	110.60
1	B	42[B]	ASP	N-CA-CB	5.07	119.73	110.60
1	B	89	ASP	CB-CG-OD2	-5.06	113.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	ASP	OD1-CG-OD2	-5.04	113.72	123.30
1	A	9	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	LEU	Mainchain
1	A	4	ASN	Mainchain
1	A	5[B]	TYR	Mainchain
1	A	92	GLU	Sidechain
1	B	136[A]	TYR	Sidechain
1	B	177	LEU	Mainchain
1	B	4	ASN	Mainchain
1	B	5[B]	TYR	Mainchain
1	B	95	GLU	Sidechain

## 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	1491	0	1454	23	0
1	B	1484	0	1444	23	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	270	0	0	4	1
3	B	285	0	0	6	1
All	All	3534	0	2898	44	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 7.

All (44) 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:16[A]:PHE:CE2	1:A:100:VAL:HG22	1.32	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16[B]:PHE:CE1	1:B:100:VAL:HG22	1.34	1.58
1:B:16[B]:PHE:HE1	1:B:100:VAL:CG2	1.31	1.41
1:A:16[A]:PHE:HE2	1:A:100:VAL:CG2	1.36	1.37
1:B:160[B]:LYS:HD3	3:B:386:HOH:O	1.11	1.28
1:A:16[A]:PHE:CE2	1:A:100:VAL:CG2	2.16	1.17
1:B:136[A]:TYR:OH	3:B:399:HOH:O	1.60	1.14
1:B:16[B]:PHE:CE1	1:B:100:VAL:CG2	2.13	1.06
1:A:16[A]:PHE:CD2	1:A:100:VAL:HG22	1.93	1.03
1:A:5[B]:TYR:HB2	3:B:437:HOH:O	1.65	0.95
1:B:16[B]:PHE:CD1	1:B:100:VAL:HG22	2.06	0.89
1:A:145[B]:GLU:CG	3:A:541:HOH:O	2.26	0.83
1:B:4:ASN:O	1:B:5[B]:TYR:HB3	1.79	0.81
1:A:5[B]:TYR:CB	3:B:437:HOH:O	2.28	0.79
1:A:145[B]:GLU:HG3	3:A:541:HOH:O	1.83	0.77
1:A:4:ASN:O	1:A:5[B]:TYR:HB3	1.89	0.72
1:B:43[B]:CYS:SG	1:B:100:VAL:HG21	2.31	0.71
1:A:16[A]:PHE:CD2	1:A:100:VAL:CG2	2.64	0.68
1:B:16[B]:PHE:CD1	1:B:100:VAL:CG2	2.74	0.63
1:B:16[B]:PHE:CE1	1:B:100:VAL:HG23	2.27	0.62
1:A:16[A]:PHE:HE2	1:A:100:VAL:CB	2.11	0.60
1:A:43[B]:CYS:SG	1:A:100:VAL:HG21	2.41	0.60
1:B:16[B]:PHE:HE1	1:B:100:VAL:CB	2.14	0.59
1:B:60:ILE:HD11	1:B:175[B]:ASN:HD21	1.69	0.58
1:A:60:ILE:HD11	1:A:175[B]:ASN:HD21	1.69	0.57
1:A:179:VAL:O	1:A:180:ALA:HB2	2.05	0.55
1:B:54:ARG:HD2	3:B:516:HOH:O	2.07	0.55
1:A:145[B]:GLU:CD	3:A:541:HOH:O	2.45	0.54
1:A:11[A]:MET:SD	1:A:110:VAL:HG22	2.49	0.52
1:A:17:PHE:CE1	1:A:127:VAL:HA	2.44	0.52
1:A:10:PHE:CE1	1:A:11[B]:MET:HG2	2.44	0.51
1:B:43[B]:CYS:SG	1:B:100:VAL:HG11	2.51	0.51
1:B:17:PHE:CE1	1:B:127:VAL:HA	2.47	0.48
1:B:11[A]:MET:SD	1:B:110:VAL:HG22	2.53	0.48
1:B:53[B]:ARG:HH11	1:B:54:ARG:NH2	2.11	0.48
1:A:43[B]:CYS:SG	1:A:100:VAL:HG11	2.55	0.47
1:A:16[A]:PHE:CE2	1:A:100:VAL:HG23	2.37	0.47
1:B:34:ILE:HD13	1:B:79[A]:THR:HG22	1.97	0.46
1:B:160[B]:LYS:HE3	3:B:277:HOH:O	2.16	0.45
1:A:177:LEU:HD13	1:B:174:GLU:HA	1.99	0.45
1:B:53[B]:ARG:HH11	1:B:54:ARG:HH22	1.65	0.44
1:A:145[B]:GLU:OE2	3:A:541:HOH:O	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLU:HA	1:B:177:LEU:HD13	2.02	0.41
1:B:3:LEU:O	1:B:4:ASN:HB2	2.22	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)
3:A:265:HOH:O	3:B:445:HOH:O[2_665]	2.18	0.02

## 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	194/179 (108%)	186 (96%)	5 (3%)	3 (2%)	12	1
1	B	194/179 (108%)	185 (95%)	6 (3%)	3 (2%)	12	1
All	All	388/358 (108%)	371 (96%)	11 (3%)	6 (2%)	17	1

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	5[A]	TYR
1	A	5[B]	TYR
1	B	4	ASN
1	B	5[A]	TYR
1	B	5[B]	TYR

### 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	160/146 (110%)	157 (98%)	3 (2%)	62	21
1	B	159/146 (109%)	157 (99%)	2 (1%)	73	35
All	All	319/292 (109%)	314 (98%)	5 (2%)	64	29

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	54	ARG
1	A	107	ILE
1	B	3	LEU
1	B	107	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	B	4	ASN
1	B	23	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 4 ligands modelled in this entry, 4 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 [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, 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	179/179 (100%)	-0.25	6 (3%)	46	43	6, 10, 27, 42	0
1	B	179/179 (100%)	-0.28	6 (3%)	46	43	6, 10, 26, 35	0
All	All	358/358 (100%)	-0.26	12 (3%)	46	43	6, 10, 27, 42	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	ALA	9.4
1	A	180	ALA	8.4
1	A	2	GLY	6.0
1	B	3	LEU	5.8
1	A	3	LEU	5.6
1	B	179	VAL	4.5
1	A	179	VAL	4.5
1	B	4	ASN	4.2
1	A	4	ASN	4.1
1	B	2	GLY	3.7
1	A	5[A]	TYR	2.4
1	B	5[A]	TYR	2.3

### 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(Å <sup>2</sup> )	Q<0.9
2	FE	A	182	1/1	1.00	0.04	-1.96	5,5,5,5	0
2	FE	B	182	1/1	1.00	0.05	-2.24	5,5,5,5	0
2	FE	B	181	1/1	1.00	0.03	-3.78	7,7,7,7	0
2	FE	A	181	1/1	1.00	0.03	-4.88	7,7,7,7	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.