



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 22, 2018 – 09:00 PM EST

PDB ID : 6B58  
Title : FrdA-SdhE assembly intermediate  
Authors : Sharma, P.; Iverson, T.M.  
Deposited on : 2017-09-28  
Resolution : 2.61 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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
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-20030736

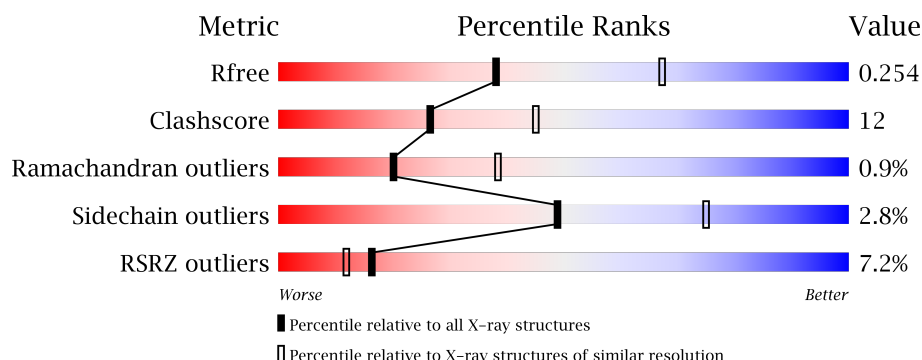
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	2983 (2.64-2.60)
Clashscore	112137	3351 (2.64-2.60)
Ramachandran outliers	110173	3298 (2.64-2.60)
Sidechain outliers	110143	3298 (2.64-2.60)
RSRZ outliers	101464	2992 (2.64-2.60)

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	577	<div> <div>4%</div> <div>68%</div> <div>24%</div> <div>6%</div> </div>
1	C	577	<div> <div>2%</div> <div>75%</div> <div>18%</div> <div>6%</div> </div>
2	B	79	<div> <div>38%</div> <div>76%</div> <div>23%</div> <div>.</div> </div>
2	D	79	<div> <div>33%</div> <div>68%</div> <div>27%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	A	606	-	-	-	X
5	ACT	A	607	-	-	X	-
5	ACT	A	608	-	-	X	-
5	ACT	C	609	-	-	X	X
6	EDO	A	610	-	-	-	X
6	EDO	A	611	-	-	-	X
8	MLI	C	604	-	-	X	-
9	GOL	C	605	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9567 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 Fumarate reductase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	542	Total	C	N	O	S	0	1	0
			4135	2583	738	785	29			
1	C	544	Total	C	N	O	S	0	0	0
			4100	2556	736	778	30			

- Molecule 2 is a protein called FAD assembly factor SdhE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	79	Total	C	N	O	S	0	0	0
			538	328	99	104	7			
2	D	78	Total	C	N	O	S	0	0	0
			543	338	105	95	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	PBF	ARG	engineered mutation	UNP P64561
D	8	PBF	ARG	engineered mutation	UNP P64561

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	C	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



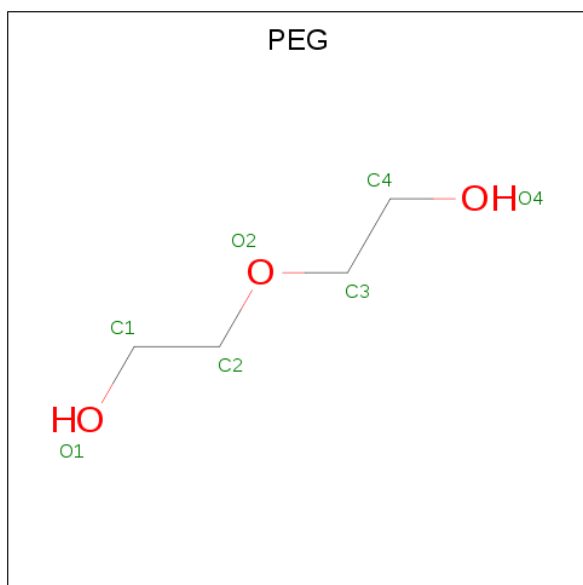
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



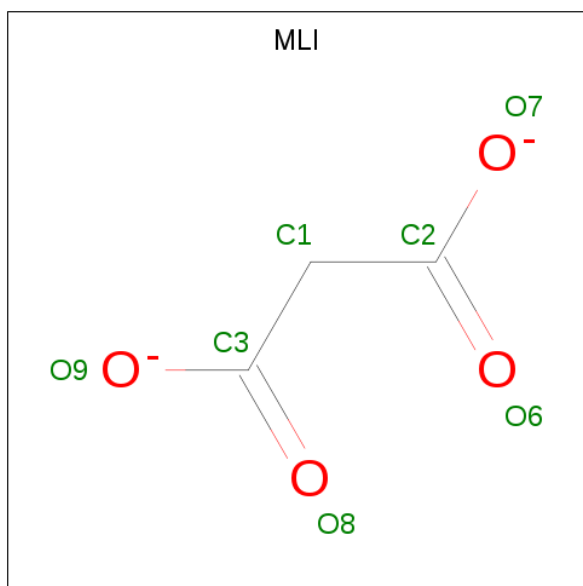
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



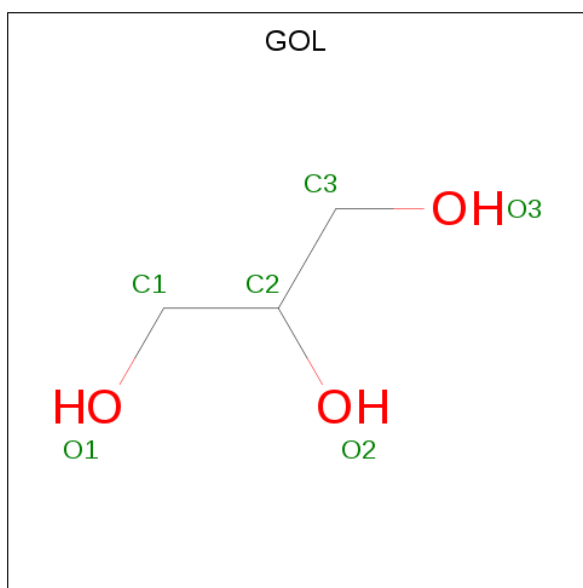
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			7	3	4		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			6	3	3		

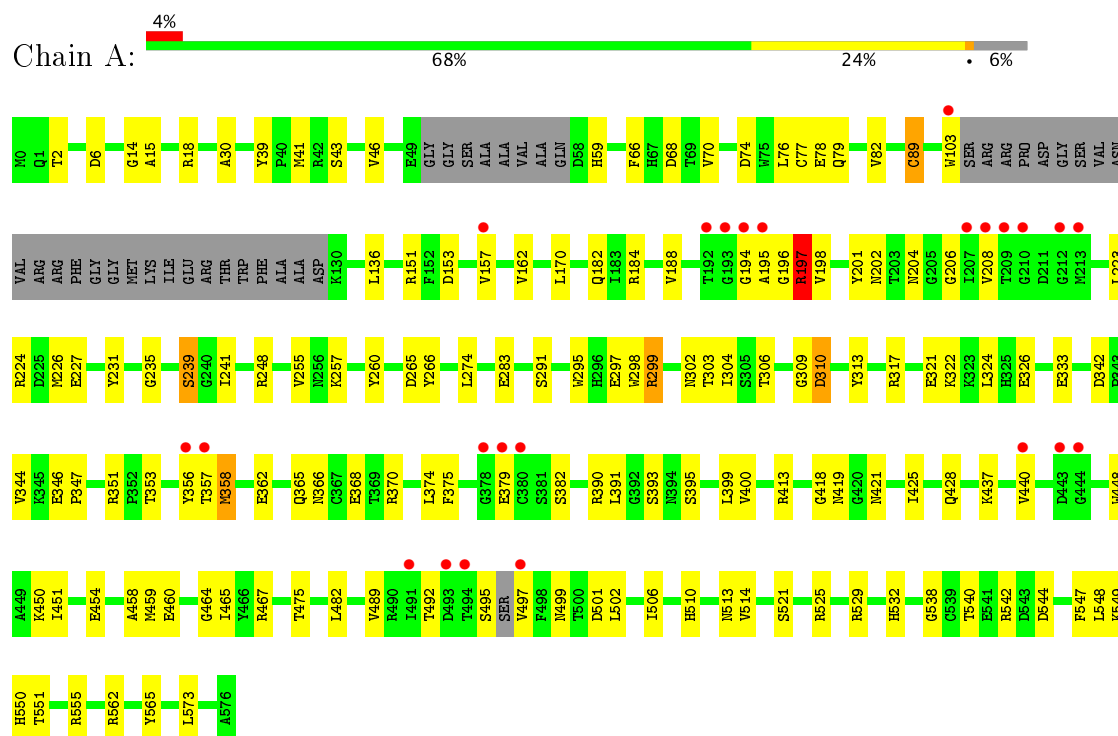
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	29	Total	O	0	0
			29	29		
10	B	1	Total	O	0	0
			1	1		
10	C	33	Total	O	0	0
			33	33		

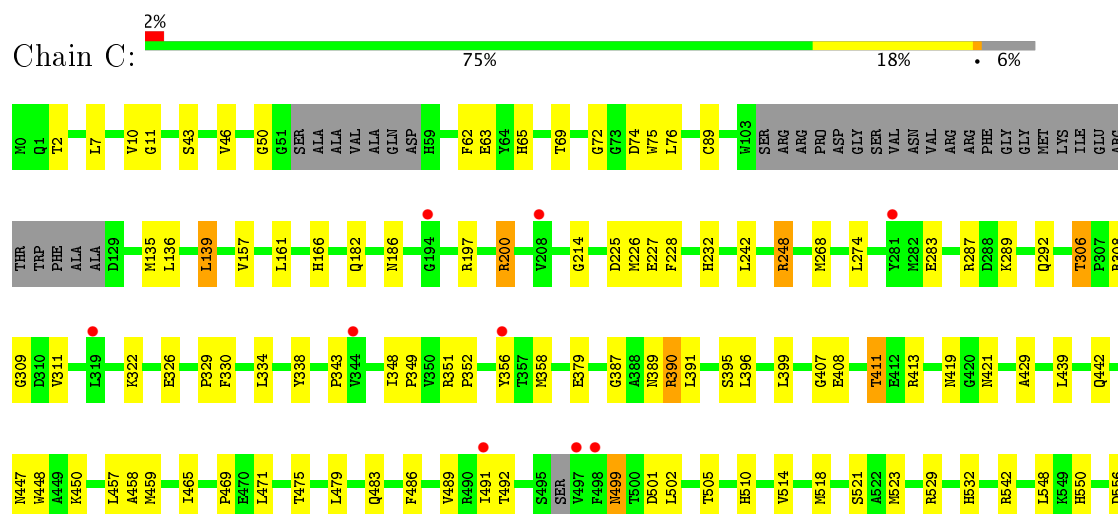
### 3 Residue-property plots

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: Fumarate reductase flavoprotein subunit

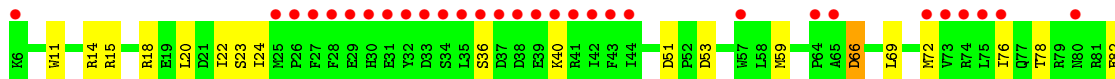
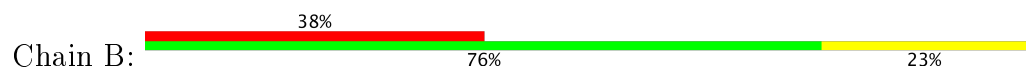


#### • Molecule 1: Fumarate reductase flavoprotein subunit

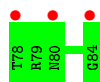
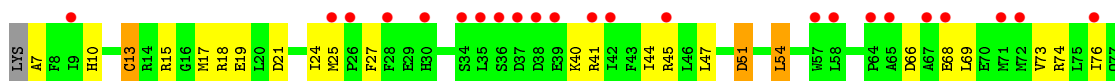




• Molecule 2: FAD assembly factor SdhE



• Molecule 2: FAD assembly factor SdhE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.64Å 63.33Å 175.58Å 90.00° 96.83° 90.00°	Depositor
Resolution (Å)	37.15 – 2.61 37.15 – 2.61	Depositor EDS
% Data completeness (in resolution range)	96.2 (37.15-2.61) 96.2 (37.15-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.191 , 0.255 0.190 , 0.254	Depositor DCC
$R_{free}$ test set	2025 reflections (4.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.2	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, K, MLI, EDO, PBF, ACT, PEG, FAD

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	0.49	1/4220 (0.0%)	0.64	0/5712
1	C	0.50	1/4181 (0.0%)	0.65	1/5665 (0.0%)
2	B	0.35	0/539	0.52	0/729
2	D	0.35	0/547	0.53	0/742
All	All	0.48	2/9487 (0.0%)	0.64	1/12848 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	89	CYS	CB-SG	-6.20	1.71	1.82
1	A	89	CYS	CB-SG	-5.42	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	LEU	CB-CG-CD2	-5.03	102.45	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	4135	0	3986	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4100	0	3910	72	0
2	B	538	0	424	13	0
2	D	543	0	448	21	0
3	A	53	0	29	1	0
3	C	53	0	29	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	28	0	21	9	0
5	C	16	0	12	4	0
6	A	16	0	24	2	0
7	C	7	0	10	0	0
8	C	7	0	2	5	0
9	C	6	0	8	0	0
10	A	29	0	0	0	0
10	B	1	0	0	0	0
10	C	33	0	0	2	0
All	All	9567	0	8903	214	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 12.

All (214) 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:346:GLU:HG3	1:A:347:PRO:HD2	1.35	1.03
2:D:13:CYS:SG	2:D:25:MET:SD	2.66	0.94
2:D:15:ARG:NH1	2:D:51:ASP:OD1	2.10	0.85
1:A:467:ARG:NH1	1:A:532:HIS:ND1	2.26	0.83
1:A:162:VAL:O	1:A:428:GLN:NE2	2.12	0.82
1:C:395:SER:O	1:C:399:LEU:HD13	1.81	0.80
1:A:15:ALA:HB2	1:A:399:LEU:HD22	1.62	0.80
1:A:197:ARG:NH2	2:B:18:ARG:NE	2.33	0.76
1:A:358:MET:CE	1:A:390:ARG:H	2.00	0.75
1:A:366:ASN:ND2	5:A:603:ACT:O	2.19	0.74
1:A:303:THR:HG21	1:A:310:ASP:HB3	1.70	0.72
1:C:287:ARG:HH12	8:C:604:MLI:H12	1.56	0.70
1:A:15:ALA:HB2	1:A:399:LEU:CD2	2.22	0.70
1:C:491:ILE:HD12	1:C:502:LEU:HA	1.75	0.69
1:C:562:ARG:NH1	1:C:564:GLU:OE1	2.21	0.69
1:A:196:GLY:O	1:A:202:ASN:ND2	2.26	0.69
1:A:502:LEU:O	1:A:506:ILE:HG13	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:SER:O	1:A:46:VAL:HG22	1.93	0.68
2:D:73:VAL:HG13	2:D:74:ARG:H	1.59	0.68
1:C:556:ASP:OD2	1:C:562:ARG:HD3	1.95	0.67
1:C:50:GLY:HA3	8:C:604:MLI:O7	1.95	0.67
1:A:151:ARG:NH1	1:A:153:ASP:OD2	2.28	0.66
1:A:454:GLU:HB2	1:A:482:LEU:HD11	1.77	0.66
1:A:14:GLY:HA3	1:A:399:LEU:HD13	1.76	0.66
2:B:15:ARG:HD2	2:B:51:ASP:OD1	1.95	0.66
1:A:418:GLY:O	1:A:419:ASN:ND2	2.27	0.65
1:C:334:LEU:HD12	1:C:338:TYR:HE1	1.61	0.65
1:C:501:ASP:O	1:C:505:THR:HG23	1.96	0.65
1:C:43:SER:O	1:C:46:VAL:HG22	1.97	0.65
1:A:437:LYS:HA	1:A:440:VAL:HG22	1.79	0.64
2:D:44:ILE:HA	2:D:47:LEU:HD12	1.80	0.64
1:A:358:MET:HE3	1:A:390:ARG:H	1.61	0.64
1:A:538:GLY:H	5:A:608:ACT:H2	1.63	0.64
1:A:391:LEU:HD12	5:A:607:ACT:H3	1.81	0.63
2:D:10:HIS:HE1	2:D:25:MET:CE	2.13	0.62
1:A:542:ARG:NH1	1:A:544:ASP:OD1	2.33	0.62
1:A:548:LEU:HD23	5:A:605:ACT:H2	1.82	0.62
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.83	0.61
1:A:257:LYS:HE2	1:A:302:ASN:HA	1.81	0.61
1:A:395:SER:OG	3:A:601:FAD:O2	2.18	0.61
1:A:197:ARG:NH2	2:B:18:ARG:HE	1.99	0.61
1:A:425:ILE:HD12	1:A:425:ILE:H	1.66	0.60
1:C:407:GLY:O	1:C:411:THR:HG22	2.01	0.60
1:C:352:PRO:HB2	1:C:465:ILE:HD11	1.83	0.59
1:A:194:GLY:O	1:A:208:VAL:HG12	2.02	0.59
2:D:17:MET:HB3	2:D:19:GLU:OE2	2.02	0.59
2:D:13:CYS:HB2	2:D:24:ILE:HG22	1.85	0.59
1:A:346:GLU:HG3	1:A:347:PRO:CD	2.23	0.58
1:C:458:ALA:HB1	1:C:475:THR:HG23	1.84	0.58
1:A:299:ARG:NH1	6:A:611:EDO:H11	2.18	0.58
1:A:448:TRP:HB3	1:A:489:VAL:HG21	1.88	0.56
1:A:358:MET:HE3	1:A:390:ARG:HB3	1.86	0.56
1:A:451:ILE:HG23	1:A:482:LEU:HD22	1.88	0.55
1:C:69:THR:HA	1:C:391:LEU:HD11	1.88	0.55
1:C:166:HIS:HE1	1:C:186:ASN:O	1.89	0.55
1:C:390:ARG:HD2	1:C:395:SER:HB3	1.88	0.55
1:A:538:GLY:N	5:A:608:ACT:H2	2.21	0.55
1:C:287:ARG:NH1	8:C:604:MLI:H12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:GLN:NE2	5:C:608:ACT:O	2.40	0.55
1:A:358:MET:HE3	1:A:390:ARG:CB	2.36	0.54
1:C:343:PRO:HG3	1:C:348:ILE:HD11	1.89	0.54
1:C:459:MET:CE	1:C:479:LEU:HD11	2.37	0.54
1:A:239:SER:HB2	1:A:241:ILE:HG13	1.87	0.54
1:C:447:ASN:OD1	1:C:450:LYS:N	2.38	0.54
1:A:196:GLY:C	1:A:202:ASN:HD21	2.10	0.54
1:A:540:THR:OG1	5:A:608:ACT:H3	2.07	0.54
1:A:66:PHE:CZ	1:A:79:GLN:HG2	2.42	0.54
1:A:368:GLU:OE1	1:A:413:ARG:NE	2.41	0.54
1:A:224:ARG:HD2	1:A:382:SER:OG	2.09	0.53
1:A:74:ASP:O	1:A:529:ARG:NH1	2.40	0.53
1:A:196:GLY:O	1:A:198:VAL:N	2.41	0.53
2:B:23:SER:O	2:B:76:ILE:HD11	2.07	0.53
2:B:72:MET:O	2:B:76:ILE:HG22	2.09	0.53
1:C:486:PHE:O	1:C:489:VAL:HG23	2.08	0.53
1:C:459:MET:HE3	1:C:479:LEU:HD11	1.90	0.53
1:C:334:LEU:HD12	1:C:338:TYR:CE1	2.41	0.52
1:A:492:THR:O	1:A:499:ASN:ND2	2.42	0.52
1:A:303:THR:HG22	1:A:304:ILE:H	1.73	0.52
1:A:227:GLU:OE2	1:A:525:ARG:NE	2.39	0.52
1:A:333:GLU:HG3	2:B:59:MET:O	2.08	0.52
1:C:408:GLU:O	1:C:411:THR:HG23	2.10	0.52
1:A:298:TRP:HA	1:A:303:THR:OG1	2.10	0.52
2:B:18:ARG:CZ	2:B:22:ILE:HD11	2.40	0.52
1:A:197:ARG:HG3	1:A:206:GLY:HA2	1.93	0.51
1:A:375:PHE:HZ	1:A:413:ARG:HD2	1.76	0.51
1:A:495:SER:O	1:A:497:VAL:N	2.43	0.51
1:C:306:THR:HG22	1:C:309:GLY:N	2.26	0.51
2:D:66:ASP:OD1	2:D:68:GLU:N	2.33	0.51
1:A:46:VAL:HG13	1:A:136:LEU:HD23	1.91	0.51
1:A:391:LEU:HD12	5:A:607:ACT:CH3	2.41	0.51
1:C:248:ARG:HG2	1:C:283:GLU:HB3	1.93	0.51
1:C:287:ARG:HH12	8:C:604:MLI:C1	2.23	0.51
2:B:20:LEU:HB3	2:B:24:ILE:HD13	1.92	0.51
1:A:196:GLY:C	1:A:198:VAL:H	2.13	0.50
1:A:306:THR:HG22	1:A:309:GLY:O	2.10	0.50
1:A:15:ALA:CB	1:A:399:LEU:HD22	2.38	0.50
1:C:448:TRP:HB3	1:C:489:VAL:HG11	1.94	0.50
2:D:10:HIS:CE1	2:D:25:MET:CE	2.94	0.50
1:C:62:PHE:HB3	5:C:609:ACT:H1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ARG:CZ	1:A:542:ARG:HD2	2.43	0.49
1:A:521:SER:HB3	1:A:551:THR:HG21	1.94	0.49
1:C:483:GLN:HG2	10:C:702:HOH:O	2.12	0.49
1:A:299:ARG:HH12	6:A:611:EDO:H11	1.77	0.49
1:C:10:VAL:HG13	1:C:157:VAL:HG21	1.93	0.49
1:C:532:HIS:HA	10:C:712:HOH:O	2.13	0.49
1:A:78:GLU:O	1:A:82:VAL:HG23	2.12	0.49
1:A:59:HIS:HE1	1:A:89:CYS:HB2	1.77	0.48
1:C:214:GLY:HA3	1:C:510:HIS:ND1	2.27	0.48
1:C:135:MET:O	1:C:139:LEU:HD22	2.12	0.48
1:C:65:HIS:O	1:C:69:THR:HG23	2.12	0.48
2:B:36:SER:HA	2:B:40:LYS:HG3	1.94	0.48
1:A:231:TYR:OH	1:A:464:GLY:HA2	2.14	0.48
1:C:161:LEU:HD11	1:C:429:ALA:HB2	1.96	0.48
1:A:362:GLU:OE1	1:A:370:ARG:NH1	2.46	0.48
1:A:255:VAL:HA	1:A:260:TYR:O	2.14	0.48
1:C:457:LEU:HA	1:C:457:LEU:HD23	1.62	0.47
1:A:358:MET:HE2	1:A:390:ARG:H	1.75	0.47
2:D:73:VAL:HG13	2:D:74:ARG:N	2.27	0.47
2:D:40:LYS:O	2:D:44:ILE:HG13	2.15	0.47
1:A:195:ALA:H	1:A:357:THR:HG21	1.80	0.47
1:A:499:ASN:ND2	1:A:501:ASP:HB2	2.30	0.47
1:C:72:GLY:O	1:C:389:ASN:HB3	2.14	0.47
1:C:11:GLY:HA2	3:C:601:FAD:H1B	1.96	0.47
1:A:235:GLY:HA3	1:A:353:THR:OG1	2.15	0.46
1:C:514:VAL:O	1:C:518:MET:HG3	2.15	0.46
1:A:151:ARG:HH11	1:A:153:ASP:CG	2.19	0.46
1:A:196:GLY:HA3	1:A:204:ASN:ND2	2.29	0.46
2:D:10:HIS:HE1	2:D:25:MET:HE3	1.81	0.46
1:A:313:TYR:HB3	1:A:347:PRO:HB2	1.98	0.46
1:C:396:LEU:O	1:C:399:LEU:HB2	2.14	0.46
1:C:69:THR:HA	1:C:391:LEU:CD1	2.46	0.46
2:B:78:THR:O	2:B:82:GLU:HG3	2.14	0.46
1:A:510:HIS:O	1:A:514:VAL:HG13	2.15	0.46
1:C:74:ASP:HB3	1:C:529:ARG:HG2	1.97	0.46
2:B:15:ARG:HA	2:B:15:ARG:HD3	1.75	0.45
2:D:66:ASP:HB3	2:D:69:LEU:CB	2.46	0.45
1:A:76:LEU:HD11	1:A:549:LYS:O	2.17	0.45
1:A:538:GLY:H	5:A:608:ACT:CH3	2.29	0.45
1:C:232:HIS:CD2	1:C:242:LEU:HD11	2.52	0.45
1:A:182:GLN:OE1	1:A:184:ARG:NE	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:VAL:HG13	1:C:136:LEU:HD23	1.99	0.45
1:A:248:ARG:HG2	1:A:283:GLU:HB3	1.98	0.45
1:A:550:HIS:O	1:A:565:TYR:HA	2.17	0.44
1:C:274:LEU:HA	1:C:274:LEU:HD12	1.87	0.44
1:C:558:ASP:OD2	1:C:560:THR:HG22	2.17	0.44
1:A:321:GLU:HA	1:A:324:LEU:HB2	1.99	0.44
1:A:413:ARG:HG3	1:A:413:ARG:HH11	1.83	0.44
2:D:41:ARG:HA	2:D:44:ILE:HD11	2.00	0.44
1:C:2:THR:HA	1:C:182:GLN:O	2.18	0.44
2:D:69:LEU:O	2:D:73:VAL:HG12	2.17	0.44
1:C:227:GLU:HG3	1:C:521:SER:HB3	1.99	0.44
2:D:51:ASP:HA	2:D:54:LEU:HD12	2.00	0.44
2:D:44:ILE:HD12	2:D:45:ARG:N	2.33	0.44
1:C:356:TYR:CZ	1:C:379:GLU:HG3	2.53	0.43
1:A:6:ASP:OD2	1:A:30:ALA:HA	2.18	0.43
1:A:317:ARG:CZ	1:A:347:PRO:HD3	2.48	0.43
1:C:200:ARG:NH2	1:C:457:LEU:HG	2.33	0.43
1:C:63:GLU:HA	5:C:609:ACT:H2	1.99	0.43
1:A:391:LEU:CD1	5:A:607:ACT:H3	2.47	0.43
1:A:39:TYR:CE2	1:A:41:MET:HB2	2.54	0.43
1:A:548:LEU:HD12	1:A:548:LEU:HA	1.89	0.43
1:A:356:TYR:CE1	1:A:379:GLU:HG3	2.53	0.43
1:C:197:ARG:HH12	2:D:18:ARG:NH1	2.17	0.43
1:C:268:MET:HE2	1:C:289:LYS:HB3	2.01	0.43
2:B:11:TRP:CH2	2:B:14:ARG:NH1	2.87	0.43
1:C:306:THR:HG22	1:C:309:GLY:H	1.84	0.43
1:A:2:THR:HB	1:A:182:GLN:HB3	2.00	0.42
1:A:547:PHE:O	1:A:549:LYS:N	2.51	0.42
1:A:513:ASN:HD22	1:A:555:ARG:HD2	1.83	0.42
1:C:311:VAL:HG11	1:C:349:PRO:HB3	2.01	0.42
1:A:266:TYR:OH	1:A:297:GLU:OE2	2.32	0.42
1:C:306:THR:HG23	1:C:308:ARG:H	1.84	0.42
1:A:321:GLU:OE2	1:A:322:LYS:N	2.52	0.42
1:A:342:ASP:OD1	1:A:344:VAL:HG12	2.19	0.42
1:A:68:ASP:O	1:A:391:LEU:HD13	2.19	0.42
1:C:469:PRO:O	1:C:523:MET:HE1	2.19	0.42
1:C:76:LEU:O	1:C:387:GLY:HA2	2.18	0.42
1:A:223:LEU:HB3	1:A:226:MET:CG	2.49	0.42
1:C:225:ASP:HB3	1:C:228:PHE:HD1	1.84	0.42
1:C:439:LEU:O	1:C:442:GLN:HB3	2.20	0.42
1:A:260:TYR:HE2	1:A:265:ASP:OD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:TYR:HB2	1:A:460:GLU:OE1	2.20	0.42
1:A:513:ASN:HD22	1:A:555:ARG:CD	2.33	0.42
1:C:46:VAL:HG13	1:C:136:LEU:CD2	2.50	0.42
1:A:450:LYS:O	1:A:454:GLU:HG3	2.20	0.42
1:A:274:LEU:HD12	1:A:274:LEU:HA	1.81	0.41
1:C:550:HIS:O	1:C:565:TYR:HA	2.20	0.41
1:A:303:THR:HG22	1:A:304:ILE:N	2.35	0.41
2:D:27:PHE:CE2	2:D:76:ILE:HG12	2.55	0.41
1:A:70:VAL:HA	1:A:77:CYS:SG	2.61	0.41
1:C:499:ASN:O	1:C:502:LEU:N	2.35	0.41
2:B:66:ASP:O	2:B:69:LEU:N	2.31	0.41
1:C:471:LEU:HA	1:C:471:LEU:HD12	1.90	0.41
1:A:573:LEU:HA	1:A:573:LEU:HD23	1.93	0.41
1:A:157:VAL:HG13	1:A:170:LEU:HD13	2.02	0.41
1:A:304:ILE:HD13	1:A:313:TYR:CE2	2.55	0.41
1:A:304:ILE:HD13	1:A:313:TYR:CZ	2.55	0.41
2:D:21:ASP:O	2:D:25:MET:HB3	2.21	0.41
1:A:46:VAL:HG13	1:A:136:LEU:CD2	2.51	0.41
1:A:295:TRP:O	1:A:298:TRP:HB3	2.21	0.41
1:A:2:THR:HA	1:A:182:GLN:O	2.21	0.41
1:A:321:GLU:N	1:A:321:GLU:OE2	2.54	0.41
1:C:330:PHE:O	1:C:334:LEU:HB2	2.21	0.41
1:C:395:SER:OG	3:C:601:FAD:O2	2.32	0.41
1:C:63:GLU:HG3	5:C:609:ACT:H2	2.03	0.41
1:C:529:ARG:HG3	1:C:542:ARG:HG3	2.02	0.41
1:A:291:SER:HB3	1:A:465:ILE:HD12	2.01	0.40
1:C:228:PHE:O	1:C:358:MET:HB2	2.21	0.40
1:C:390:ARG:HH22	8:C:604:MLI:C3	2.34	0.40
2:D:7:ALA:HB1	2:D:10:HIS:HD2	1.86	0.40
1:A:151:ARG:NH1	1:A:153:ASP:CG	2.74	0.40
1:A:458:ALA:O	1:A:475:THR:HG21	2.21	0.40
1:C:226:MET:HB3	1:C:518:MET:HG2	2.02	0.40
1:A:188:VAL:O	1:A:374:LEU:HD12	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	535/577 (93%)	501 (94%)	31 (6%)	3 (1%)	28	51
1	C	536/577 (93%)	495 (92%)	34 (6%)	7 (1%)	14	27
2	B	76/79 (96%)	58 (76%)	17 (22%)	1 (1%)	14	27
2	D	75/79 (95%)	66 (88%)	9 (12%)	0	100	100
All	All	1222/1312 (93%)	1120 (92%)	91 (7%)	11 (1%)	20	38

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	326	GLU
1	C	499	ASN
1	A	421	ASN
2	B	66	ASP
1	A	197	ARG
1	C	421	ASN
1	C	548	LEU
1	C	322	LYS
1	C	329	PRO
1	A	326	GLU
1	C	492	THR

### 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	422/460 (92%)	411 (97%)	11 (3%)	51	77
1	C	411/460 (89%)	400 (97%)	11 (3%)	50	76
2	B	41/71 (58%)	40 (98%)	1 (2%)	54	78
2	D	41/71 (58%)	38 (93%)	3 (7%)	16	32
All	All	915/1062 (86%)	889 (97%)	26 (3%)	49	75

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	TRP
1	A	197	ARG
1	A	239	SER
1	A	299	ARG
1	A	310	ASP
1	A	351	ARG
1	A	358	MET
1	A	365	GLN
1	A	393	SER
1	A	459	MET
1	A	562	ARG
2	B	53	ASP
1	C	75	TRP
1	C	139	LEU
1	C	200	ARG
1	C	248	ARG
1	C	306	THR
1	C	351	ARG
1	C	390	ARG
1	C	411	THR
1	C	413	ARG
1	C	419	ASN
1	C	573	LEU
2	D	13	CYS
2	D	51	ASP
2	D	54	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS

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Mol	Chain	Res	Type
1	A	419	ASN
1	A	483	GLN
1	A	513	ASN
2	D	10	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PBF	B	8	2	4,4,21	1.11	0	1,4,28	0.20	0
2	PBF	D	8	2	4,4,21	1.23	1 (25%)	1,4,28	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PBF	B	8	2	-	0/0/2/16	0/0/0/2
2	PBF	D	8	2	-	0/0/2/16	0/0/0/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	8	PBF	CA-C	2.18	1.53	1.50

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.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	FAD	A	601	1	51,58,58	1.03	5 (9%)	54,89,89	2.27	6 (11%)
5	ACT	A	603	-	1,3,3	1.96	0	0,3,3	0.00	-
5	ACT	A	604	-	1,3,3	2.61	1 (100%)	0,3,3	0.00	-
5	ACT	A	605	-	1,3,3	1.35	0	0,3,3	0.00	-
5	ACT	A	606	-	1,3,3	1.93	0	0,3,3	0.00	-
5	ACT	A	607	-	1,3,3	1.15	0	0,3,3	0.00	-
5	ACT	A	608	-	1,3,3	1.01	0	0,3,3	0.00	-
5	ACT	A	609	-	1,3,3	2.46	1 (100%)	0,3,3	0.00	-
6	EDO	A	610	-	3,3,3	0.63	0	2,2,2	0.58	0
6	EDO	A	611	-	3,3,3	0.54	0	2,2,2	0.25	0
6	EDO	A	612	-	3,3,3	0.55	0	2,2,2	0.27	0
6	EDO	A	613	-	3,3,3	0.59	0	2,2,2	0.10	0
3	FAD	C	601	1	51,58,58	1.92	16 (31%)	54,89,89	2.22	11 (20%)
7	PEG	C	603	-	6,6,6	0.49	0	5,5,5	0.74	0
8	MLI	C	604	-	0,6,6	0.00	-	0,7,7	0.00	-
9	GOL	C	605	-	5,5,5	0.37	0	5,5,5	0.45	0
5	ACT	C	606	-	1,3,3	1.88	0	0,3,3	0.00	-
5	ACT	C	607	-	1,3,3	1.91	0	0,3,3	0.00	-
5	ACT	C	608	-	1,3,3	1.76	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ACT	C	609	-	1,3,3	0.36	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	601	1	-	0/28/50/50	0/6/6/6
5	ACT	A	603	-	-	0/0/0/0	0/0/0/0
5	ACT	A	604	-	-	0/0/0/0	0/0/0/0
5	ACT	A	605	-	-	0/0/0/0	0/0/0/0
5	ACT	A	606	-	-	0/0/0/0	0/0/0/0
5	ACT	A	607	-	-	0/0/0/0	0/0/0/0
5	ACT	A	608	-	-	0/0/0/0	0/0/0/0
5	ACT	A	609	-	-	0/0/0/0	0/0/0/0
6	EDO	A	610	-	-	0/1/1/1	0/0/0/0
6	EDO	A	611	-	-	0/1/1/1	0/0/0/0
6	EDO	A	612	-	-	0/1/1/1	0/0/0/0
6	EDO	A	613	-	-	0/1/1/1	0/0/0/0
3	FAD	C	601	1	-	0/28/50/50	0/6/6/6
7	PEG	C	603	-	-	0/4/4/4	0/0/0/0
8	MLI	C	604	-	-	0/0/4/4	0/0/0/0
9	GOL	C	605	-	-	0/4/4/4	0/0/0/0
5	ACT	C	606	-	-	0/0/0/0	0/0/0/0
5	ACT	C	607	-	-	0/0/0/0	0/0/0/0
5	ACT	C	608	-	-	0/0/0/0	0/0/0/0
5	ACT	C	609	-	-	0/0/0/0	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	FAD	C1'-N10	-4.64	1.43	1.48
3	C	601	FAD	C2-N3	-3.95	1.30	1.38
3	C	601	FAD	C6-C5X	-3.82	1.36	1.41
3	C	601	FAD	C2-N1	-3.01	1.32	1.38
3	C	601	FAD	PA-O2A	-2.87	1.40	1.55
3	C	601	FAD	P-O1P	-2.84	1.40	1.50
3	C	601	FAD	P-O2P	-2.81	1.41	1.55
3	C	601	FAD	C2B-C1B	-2.79	1.49	1.53
3	C	601	FAD	PA-O1A	-2.61	1.41	1.50
3	C	601	FAD	C5A-N7A	-2.54	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	FAD	C4A-N3A	-2.43	1.32	1.35
3	C	601	FAD	C9-C9A	-2.10	1.36	1.40
3	A	601	FAD	C4X-N5	-2.08	1.30	1.33
3	C	601	FAD	O4B-C4B	-2.05	1.40	1.45
3	C	601	FAD	C2'-C3'	-2.03	1.49	1.53
3	C	601	FAD	C8-C7	2.00	1.46	1.41
3	A	601	FAD	C4-C4X	2.13	1.45	1.41
3	A	601	FAD	C9A-N10	2.20	1.41	1.38
3	C	601	FAD	C4X-C10	2.43	1.45	1.41
5	A	609	ACT	CH3-C	2.46	1.51	1.48
3	A	601	FAD	C5X-N5	2.48	1.39	1.35
5	A	604	ACT	CH3-C	2.61	1.52	1.48
3	A	601	FAD	C4-N3	3.21	1.38	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	FAD	N3A-C2A-N1A	-6.54	123.16	128.86
3	A	601	FAD	C4X-C4-N3	-6.49	114.25	123.48
3	C	601	FAD	C4-C4X-C10	-6.24	114.91	119.96
3	A	601	FAD	C4X-C10-N10	-5.39	116.78	120.52
3	C	601	FAD	C4X-C10-N10	-3.49	118.10	120.52
3	A	601	FAD	C4-C4X-C10	-3.17	117.40	119.96
3	C	601	FAD	C4X-C4-N3	-2.83	119.46	123.48
3	C	601	FAD	O3'-C3'-C2'	-2.29	103.15	108.82
3	C	601	FAD	O2'-C2'-C3'	-2.24	103.53	109.09
3	C	601	FAD	C1'-N10-C9A	2.02	120.20	118.35
3	A	601	FAD	C1'-N10-C9A	2.65	120.78	118.35
3	C	601	FAD	C5X-C9A-N10	2.81	119.75	117.66
3	C	601	FAD	C4X-N5-C5X	3.45	120.41	116.76
3	A	601	FAD	C10-C4X-N5	3.51	124.63	120.59
3	C	601	FAD	C4-C4X-N5	4.01	123.08	118.68
3	C	601	FAD	C4-N3-C2	8.50	122.59	115.16
3	A	601	FAD	C4-N3-C2	12.47	126.07	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	FAD	1	0
5	A	603	ACT	1	0
5	A	605	ACT	1	0
5	A	607	ACT	3	0
5	A	608	ACT	4	0
6	A	611	EDO	2	0
3	C	601	FAD	2	0
8	C	604	MLI	5	0
5	C	608	ACT	1	0
5	C	609	ACT	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	542/577 (93%)	0.08	24 (4%) 35 28	32, 49, 78, 108	0
1	C	544/577 (94%)	-0.04	9 (1%) 70 65	27, 47, 80, 103	0
2	B	78/79 (98%)	1.52	30 (38%) 0 0	65, 98, 116, 126	0
2	D	77/79 (97%)	1.47	26 (33%) 0 0	62, 103, 117, 119	0
All	All	1241/1312 (94%)	0.20	89 (7%) 16 12	27, 50, 103, 126	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	37	ASP	6.2
2	D	84	GLY	6.0
2	D	42	ILE	5.0
2	D	67	ALA	4.7
1	A	491	ILE	4.7
2	D	65	ALA	4.3
2	B	35	LEU	4.3
2	D	71	MET	4.2
2	D	64	PRO	4.1
2	D	36	SER	4.0
2	D	38	ASP	3.9
2	B	36	SER	3.8
2	D	41	ARG	3.7
2	B	42	ILE	3.7
2	B	57	TRP	3.6
2	D	30	HIS	3.5
1	A	209	THR	3.5
1	A	194	GLY	3.5
2	B	34	SER	3.5
2	D	78	THR	3.4
1	A	494	THR	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	80	ASN	3.3
2	D	72	MET	3.3
2	D	39	GLU	3.3
1	A	443	ASP	3.3
2	D	25	MET	3.1
1	C	491	ILE	3.1
2	B	65	ALA	3.1
2	D	35	LEU	3.1
2	B	39	GLU	3.0
2	B	76	ILE	3.0
2	B	33	ASP	3.0
1	A	193	GLY	2.9
1	A	357	THR	2.9
2	B	41	ARG	2.9
1	A	195	ALA	2.8
2	B	25	MET	2.8
1	C	319	LEU	2.8
1	A	210	GLY	2.8
2	D	34	SER	2.7
1	A	192	THR	2.7
2	D	37	ASP	2.7
2	D	28	PHE	2.6
1	C	281	TYR	2.6
2	B	28	PHE	2.6
1	A	207	ILE	2.6
1	C	498	PHE	2.6
2	B	32	TYR	2.6
1	A	444	GLY	2.5
2	B	73	VAL	2.5
2	B	30	HIS	2.5
2	D	26	PRO	2.5
1	A	379	GLU	2.5
2	D	58	LEU	2.5
2	D	68	GLU	2.5
2	B	44	ILE	2.5
2	B	43	PHE	2.4
2	B	80	ASN	2.4
1	A	356	TYR	2.3
2	D	76	ILE	2.3
2	D	57	TRP	2.3
1	C	356	TYR	2.3
1	A	208	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	213	MET	2.3
2	D	45	ARG	2.3
2	B	26	PRO	2.3
2	B	27	PHE	2.2
2	B	75	LEU	2.2
2	B	72	MET	2.2
1	A	493	ASP	2.2
1	A	497	VAL	2.2
2	B	31	GLU	2.2
2	B	74	ARG	2.2
2	B	29	GLU	2.2
1	C	194	GLY	2.2
2	B	38	ASP	2.1
1	A	157	VAL	2.1
1	A	103	TRP	2.1
1	A	380	CYS	2.1
2	D	9	ILE	2.1
1	A	378	GLY	2.1
1	C	497	VAL	2.1
1	C	344	VAL	2.1
2	B	64	PRO	2.1
2	B	40	LYS	2.1
2	B	6	LYS	2.0
1	C	208	VAL	2.0
1	A	212	GLY	2.0
1	A	440	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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	PBF	B	8	5/20	0.89	0.29	-	90,90,99,103	0
2	PBF	D	8	5/20	0.87	0.38	-	93,95,98,98	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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
6	EDO	A	610	4/4	0.90	0.30	10.60	44,47,54,54	0
9	GOL	C	605	6/6	0.79	0.23	3.59	44,49,56,61	0
5	ACT	A	606	4/4	0.83	0.26	2.10	48,58,64,70	0
6	EDO	A	611	4/4	0.88	0.22	2.10	72,73,76,76	0
5	ACT	C	609	4/4	0.93	0.29	2.01	56,60,63,69	0
5	ACT	A	604	4/4	0.85	0.21	1.02	39,57,58,58	0
7	PEG	C	603	7/7	0.85	0.21	0.74	48,51,53,68	0
8	MLI	C	604	7/7	0.87	0.21	0.56	52,58,62,64	0
6	EDO	A	612	4/4	0.86	0.21	0.40	54,57,61,61	0
5	ACT	A	607	4/4	0.94	0.21	0.37	59,61,62,64	0
5	ACT	A	608	4/4	0.94	0.15	0.11	48,64,65,67	0
3	FAD	A	601	53/53	0.97	0.26	0.01	31,41,50,58	0
4	K	A	602	1/1	0.91	0.28	-0.14	68,68,68,68	0
3	FAD	C	601	53/53	0.98	0.21	-0.29	27,37,50,58	0
5	ACT	C	608	4/4	0.93	0.14	-0.41	48,61,62,65	0
6	EDO	A	613	4/4	0.94	0.13	-1.27	49,51,53,54	0
4	K	C	602	1/1	0.97	0.10	-2.99	58,58,58,58	0
5	ACT	C	607	4/4	0.94	0.11	-	51,58,59,62	0
5	ACT	A	605	4/4	0.95	0.49	-	57,60,63,65	0
5	ACT	A	609	4/4	0.91	0.23	-	48,54,62,68	0
5	ACT	A	603	4/4	0.91	0.13	-	43,48,51,53	0
5	ACT	C	606	4/4	0.90	0.15	-	54,59,62,63	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.