



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:20 pm GMT

PDB ID : 3BI4
Title : Crystal structures of fms1 in complex with its inhibitors
Authors : Huang, Q.; Hao, Q.
Deposited on : 2007-11-29
Resolution : 2.20 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

A user guide is available at

<http://wwpdb.org/validation/2016/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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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

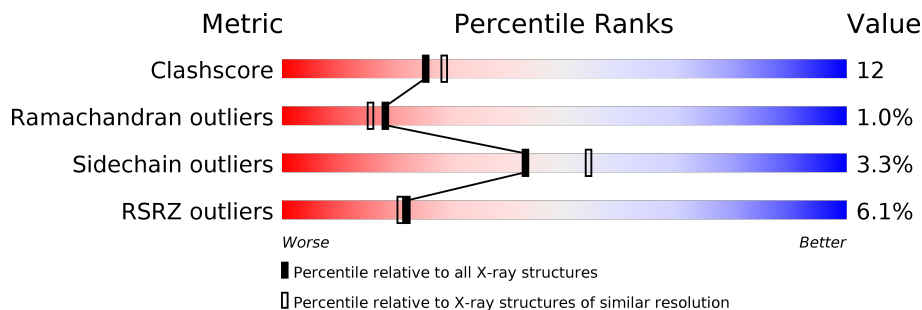
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 $\leq 5\%$. 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	516	<div> <div>5%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
1	B	516	<div> <div>7%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	298	A	1001	-	-	X	X
3	298	B	1002	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8070 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 Polyamine oxidase FMS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3889	2461	681	725	22			
1	B	496	Total	C	N	O	S	0	0	0
			3841	2423	667	729	22			

There are 16 discrepancies between the modelled and reference sequences:

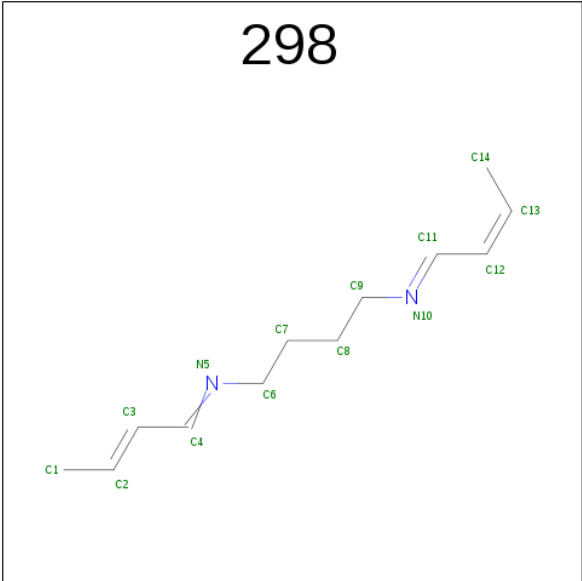
Chain	Residue	Modelled	Actual	Comment	Reference
A	509	LEU	-	EXPRESSION TAG	UNP P50264
A	510	GLU	-	EXPRESSION TAG	UNP P50264
A	511	HIS	-	EXPRESSION TAG	UNP P50264
A	512	HIS	-	EXPRESSION TAG	UNP P50264
A	513	HIS	-	EXPRESSION TAG	UNP P50264
A	514	HIS	-	EXPRESSION TAG	UNP P50264
A	515	HIS	-	EXPRESSION TAG	UNP P50264
A	516	HIS	-	EXPRESSION TAG	UNP P50264
B	509	LEU	-	EXPRESSION TAG	UNP P50264
B	510	GLU	-	EXPRESSION TAG	UNP P50264
B	511	HIS	-	EXPRESSION TAG	UNP P50264
B	512	HIS	-	EXPRESSION TAG	UNP P50264
B	513	HIS	-	EXPRESSION TAG	UNP P50264
B	514	HIS	-	EXPRESSION TAG	UNP P50264
B	515	HIS	-	EXPRESSION TAG	UNP P50264
B	516	HIS	-	EXPRESSION TAG	UNP P50264

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is N-[(1E,2Z)-BUT-2-EN-1-YLIDENE]-N'-[(2E)-BUT-2-EN-1-YLIDENE]BUTANE-1,4-DIAMINE (three-letter code: 298) (formula: C₁₂H₂₀N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			14	12	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			14	12	2		

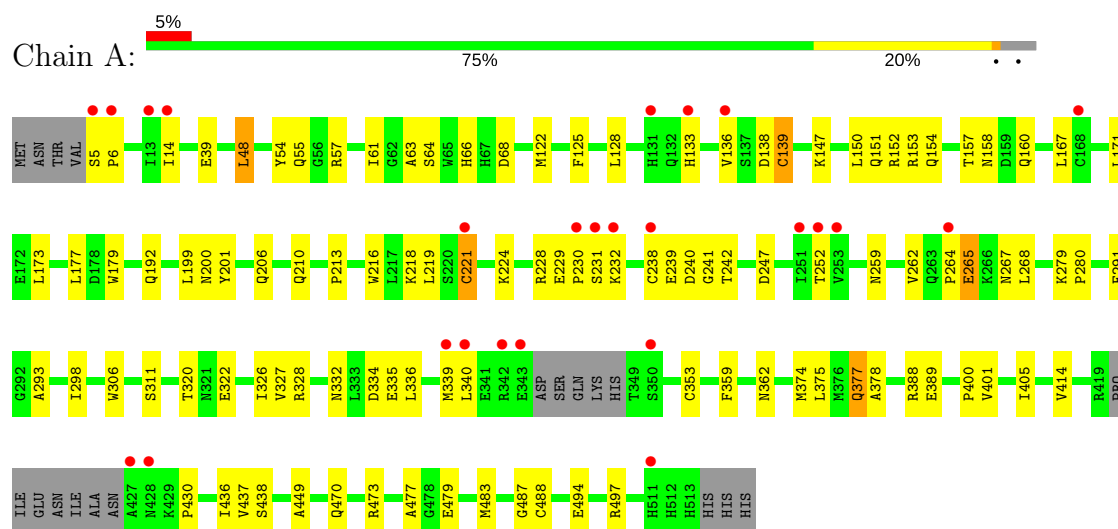
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total	O	0	0
			116	116		
4	B	90	Total	O	0	0
			90	90		

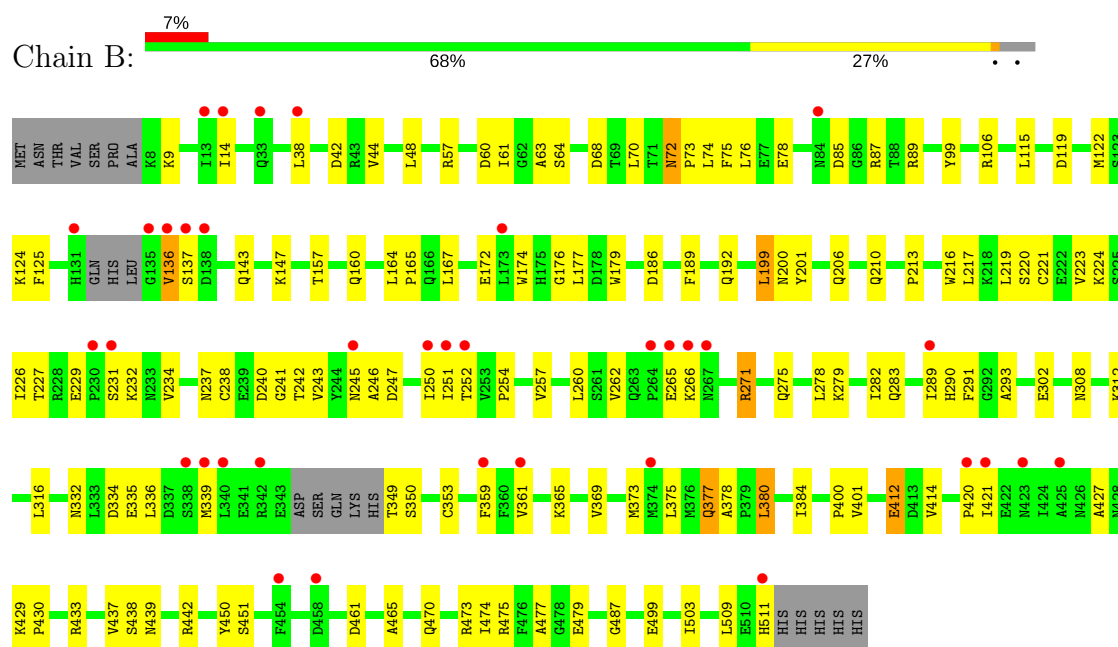
3 Residue-property plots [i](#)

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: Polyamine oxidase FMS1



• Molecule 1: Polyamine oxidase FMS1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.59Å 102.85Å 76.65Å 90.00° 94.37° 90.00°	Depositor
Resolution (Å)	32.00 – 2.20 30.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (32.00-2.20) 97.2 (30.89-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.265 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8070	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: FAD, 298

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	0.37	0/3971	0.61	2/5371 (0.0%)
1	B	0.34	0/3920	0.58	0/5304
All	All	0.36	0/7891	0.59	2/10675 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	CYS	CA-CB-SG	5.97	124.75	114.00
1	A	66	HIS	N-CA-C	-5.11	97.21	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	3889	0	3742	73	0
1	B	3841	0	3635	108	0
2	A	53	0	31	4	0
2	B	53	0	31	2	0
3	A	14	0	20	8	0
3	B	14	0	20	2	0
4	A	116	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	90	0	0	3	0
All	All	8070	0	7479	184	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 (184) 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:B:282:ILE:HD13	1:B:465:ALA:HB1	1.41	1.03
1:A:224:LYS:HD3	1:A:239:GLU:HB3	1.44	0.98
1:A:353:CYS:SG	1:A:400:PRO:HG2	2.12	0.88
1:B:377:GLN:NE2	1:B:377:GLN:H	1.75	0.83
1:B:353:CYS:SG	1:B:400:PRO:HG2	2.23	0.78
1:A:224:LYS:CD	1:A:239:GLU:HB3	2.19	0.73
1:A:240:ASP:OD1	1:A:242:THR:HG23	1.90	0.71
1:B:380:LEU:HD22	1:B:384:ILE:HG12	1.73	0.71
1:B:72:ASN:C	1:B:72:ASN:HD22	1.93	0.71
1:B:470:GLN:HB3	1:B:474:ILE:HB	1.74	0.70
1:B:479:GLU:OE1	1:B:487:GLY:HA2	1.91	0.70
1:B:473:ARG:HG3	1:B:473:ARG:HH11	1.56	0.70
1:B:439:ASN:HD21	1:B:442:ARG:HD3	1.58	0.69
1:A:320:THR:HB	1:A:322:GLU:OE2	1.93	0.69
1:B:359:PHE:HD2	1:B:375:LEU:HD22	1.58	0.68
1:B:308:ASN:O	1:B:365:LYS:HD2	1.96	0.66
1:B:335:GLU:O	1:B:339:MET:HB2	1.96	0.65
1:B:247:ASP:O	1:B:473:ARG:HD2	1.96	0.65
1:B:377:GLN:HE21	1:B:377:GLN:H	1.45	0.65
1:A:264:PRO:O	1:A:265:GLU:HB3	1.97	0.64
1:A:377:GLN:H	1:A:377:GLN:NE2	1.94	0.64
1:B:252:THR:HG22	1:B:477:ALA:HB3	1.81	0.62
1:B:219:LEU:HD12	1:B:219:LEU:N	2.14	0.62
1:A:158:ASN:ND2	1:A:328:ARG:HH21	1.97	0.62
1:B:213:PRO:HB2	1:B:216:TRP:CD1	2.34	0.62
3:A:1001:298:N10	3:A:1001:298:C14	2.59	0.62
1:A:158:ASN:HD22	1:A:328:ARG:HH21	1.47	0.61
1:A:322:GLU:O	1:A:326:ILE:HG13	2.01	0.60
1:A:229:GLU:O	1:A:231:SER:N	2.26	0.59
1:A:173:LEU:O	3:A:1001:298:H12	2.03	0.59
1:B:14:ILE:CD1	1:B:226:ILE:HD11	2.32	0.59
1:B:63:ALA:HA	2:B:802:FAD:N5	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:GLN:O	1:B:210:GLN:HG3	2.03	0.58
1:A:414:VAL:HA	1:A:430:PRO:HG2	1.85	0.58
1:A:264:PRO:O	1:A:265:GLU:CB	2.51	0.58
1:A:252:THR:HG22	1:A:477:ALA:HB3	1.85	0.57
1:B:271:ARG:HG3	1:B:271:ARG:HH11	1.69	0.57
1:B:278:LEU:HA	1:B:470:GLN:NE2	2.19	0.57
1:B:176:GLY:C	1:B:177:LEU:HD12	2.25	0.57
1:B:473:ARG:NH1	1:B:473:ARG:HG3	2.19	0.57
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.34	0.57
1:B:439:ASN:ND2	1:B:442:ARG:HD3	2.18	0.57
1:B:412:GLU:CD	1:B:429:LYS:HD2	2.25	0.57
1:B:359:PHE:CD2	1:B:375:LEU:HD22	2.40	0.56
1:A:63:ALA:HA	2:A:801:FAD:N5	2.20	0.56
1:B:72:ASN:ND2	1:B:75:PHE:H	2.04	0.56
1:B:278:LEU:HA	1:B:470:GLN:HE22	1.70	0.56
1:A:206:GLN:O	1:A:210:GLN:HG3	2.05	0.56
1:B:414:VAL:HA	1:B:430:PRO:HG2	1.88	0.55
1:A:229:GLU:C	1:A:231:SER:H	2.09	0.55
1:A:311:SER:HA	1:A:362:ASN:HB3	1.88	0.55
1:B:14:ILE:HD12	1:B:226:ILE:HD11	1.89	0.55
1:A:14:ILE:N	1:A:14:ILE:HD12	2.22	0.55
1:A:259:ASN:O	1:A:262:VAL:HG22	2.07	0.55
1:A:150:LEU:O	1:A:153:ARG:HD2	2.08	0.54
1:B:99:TYR:HB3	1:B:316:LEU:HD11	1.89	0.54
1:B:68:ASP:HB3	1:B:192:GLN:HB2	1.90	0.54
1:A:153:ARG:NH2	1:A:327:VAL:O	2.40	0.54
1:A:336:LEU:O	1:A:340:LEU:HG	2.07	0.54
1:B:271:ARG:CG	1:B:271:ARG:HH11	2.20	0.54
1:B:157:THR:OG1	1:B:160:GLN:HG3	2.08	0.54
1:B:302:GLU:HG3	1:B:433:ARG:HD3	1.89	0.54
1:B:172:GLU:HG2	1:B:177:LEU:O	2.08	0.53
1:B:232:LYS:CA	1:B:473:ARG:HH12	2.22	0.53
1:B:332:ASN:HD21	1:B:334:ASP:HB2	1.74	0.53
1:B:9:LYS:O	1:B:246:ALA:HA	2.09	0.53
1:B:260:LEU:O	1:B:271:ARG:HD2	2.09	0.53
1:A:133:HIS:HB3	1:A:136:VAL:CG2	2.39	0.52
1:A:138:ASP:O	1:A:139:CYS:SG	2.68	0.52
1:B:72:ASN:HD21	1:B:74:LEU:HB3	1.75	0.52
1:B:353:CYS:SG	1:B:401:VAL:HG13	2.50	0.52
1:B:78:GLU:OE1	1:B:89:ARG:HD3	2.10	0.52
1:B:223:VAL:HA	1:B:238:CYS:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ASP:HB3	1:B:63:ALA:O	2.09	0.51
1:A:449:ALA:HB3	4:A:1099:HOH:O	2.10	0.51
1:B:254:PRO:HG2	1:B:257:VAL:HG23	1.92	0.51
1:B:48:LEU:HD22	1:B:63:ALA:HB3	1.93	0.51
1:B:186:ASP:HB2	4:B:1060:HOH:O	2.10	0.51
1:A:133:HIS:HB3	1:A:136:VAL:HG21	1.92	0.50
1:B:213:PRO:O	1:B:216:TRP:HB2	2.11	0.50
1:A:388:ARG:NH1	1:A:437:VAL:HB	2.27	0.50
1:B:262:VAL:CG1	1:B:283:GLN:HG2	2.42	0.49
1:B:260:LEU:C	1:B:271:ARG:HD2	2.32	0.49
1:B:72:ASN:ND2	1:B:72:ASN:C	2.64	0.49
1:A:487:GLY:HA3	3:A:1001:298:C1	2.42	0.49
1:A:153:ARG:NH2	1:A:328:ARG:O	2.45	0.49
1:B:115:LEU:HB3	1:B:167:LEU:HD13	1.94	0.49
1:B:262:VAL:HG12	1:B:283:GLN:HG2	1.95	0.49
1:A:147:LYS:HE2	1:A:151:GLN:HE22	1.77	0.48
1:B:217:LEU:HG	1:B:219:LEU:CD1	2.44	0.48
1:B:254:PRO:HG2	1:B:257:VAL:CG2	2.43	0.48
1:A:232:LYS:O	1:A:473:ARG:NH1	2.46	0.48
1:A:39:GLU:HB3	1:A:219:LEU:HD23	1.96	0.48
1:B:174:TRP:CE3	1:B:189:PHE:HZ	2.31	0.48
1:A:63:ALA:HA	2:A:801:FAD:C4X	2.44	0.47
1:B:377:GLN:NE2	1:B:377:GLN:N	2.54	0.47
1:A:239:GLU:C	1:A:241:GLY:H	2.16	0.47
1:A:157:THR:OG1	1:A:160:GLN:HG3	2.15	0.47
1:B:251:ILE:HD12	1:B:251:ILE:N	2.28	0.47
1:A:298:ILE:HB	1:A:436:ILE:HB	1.96	0.47
1:B:217:LEU:CD2	1:B:219:LEU:HD11	2.45	0.47
1:B:289:ILE:O	1:B:290:HIS:HB2	2.14	0.47
1:A:48:LEU:HD22	1:A:63:ALA:HB3	1.97	0.47
1:B:164:LEU:N	1:B:165:PRO:HD2	2.30	0.47
1:B:119:ASP:O	1:B:122:MET:HB3	2.14	0.47
1:B:72:ASN:O	1:B:76:LEU:HG	2.16	0.46
1:A:332:ASN:HD21	1:A:334:ASP:HB2	1.79	0.46
1:A:68:ASP:HB3	1:A:192:GLN:HB2	1.98	0.46
1:B:475:ARG:HB3	1:B:499:GLU:OE1	2.16	0.46
1:B:450:TYR:CZ	3:B:1002:298:H7	2.51	0.45
1:B:316:LEU:N	1:B:316:LEU:HD12	2.30	0.45
1:B:420:PRO:HD3	4:B:1041:HOH:O	2.15	0.45
1:A:265:GLU:HG3	1:A:268:LEU:HG	1.98	0.45
1:A:213:PRO:HB2	1:A:216:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:MET:O	1:B:125:PHE:HB3	2.16	0.45
1:B:219:LEU:N	1:B:219:LEU:CD1	2.80	0.45
1:A:167:LEU:C	1:A:167:LEU:HD23	2.36	0.45
1:A:335:GLU:HB3	1:A:339:MET:CE	2.47	0.45
3:A:1001:298:N10	3:A:1001:298:H14A	2.32	0.45
1:A:54:TYR:O	1:A:57:ARG:HG3	2.17	0.45
1:B:136:VAL:HG23	1:B:136:VAL:O	2.17	0.45
1:B:229:GLU:O	1:B:231:SER:N	2.44	0.45
1:B:57:ARG:HD3	1:B:369:VAL:CG1	2.47	0.45
1:B:234:VAL:O	1:B:245:ASN:HA	2.17	0.44
1:A:247:ASP:O	1:A:473:ARG:HD2	2.17	0.44
1:A:128:LEU:HD21	1:B:192:GLN:OE1	2.17	0.44
1:A:335:GLU:C	1:A:339:MET:HE2	2.38	0.44
1:A:306:TRP:HE1	1:A:362:ASN:HD21	1.66	0.44
1:B:279:LYS:HE2	1:B:470:GLN:HA	2.00	0.44
1:A:488:CYS:SG	3:A:1001:298:H6A	2.58	0.44
1:B:240:ASP:OD2	1:B:242:THR:HG23	2.17	0.44
1:B:227:THR:HG23	1:B:275:GLN:HB3	2.00	0.43
1:A:280:PRO:HG2	4:A:1068:HOH:O	2.17	0.43
1:B:217:LEU:HG	1:B:219:LEU:HD11	2.00	0.43
1:B:224:LYS:HG2	1:B:237:ASN:O	2.18	0.43
1:A:359:PHE:HD2	1:A:375:LEU:HD22	1.82	0.43
1:B:85:ASP:OD1	1:B:87:ARG:N	2.45	0.43
1:A:479:GLU:OE1	1:A:487:GLY:HA2	2.19	0.43
1:B:42:ASP:OD1	1:B:42:ASP:C	2.57	0.43
1:A:5:SER:N	1:A:6:PRO:HD2	2.34	0.43
2:A:801:FAD:C4	3:A:1001:298:H9A	2.49	0.43
1:B:38:LEU:HD13	1:B:238:CYS:SG	2.59	0.43
1:B:437:VAL:HG12	1:B:438:SER:O	2.18	0.43
1:A:279:LYS:HG3	1:A:470:GLN:OE1	2.18	0.43
1:A:152:ARG:CZ	1:B:70:LEU:HD23	2.48	0.43
1:B:232:LYS:C	1:B:473:ARG:HH12	2.23	0.43
1:B:293:ALA:HB3	1:B:378:ALA:HB2	2.01	0.43
1:B:271:ARG:CG	1:B:271:ARG:NH1	2.80	0.42
1:A:293:ALA:HB3	1:A:378:ALA:HB2	2.01	0.42
1:A:494:GLU:OE1	1:A:497:ARG:NH2	2.50	0.42
1:B:237:ASN:HD22	1:B:243:VAL:HG22	1.83	0.42
1:B:61:ILE:HA	1:B:61:ILE:HD12	1.87	0.42
1:B:213:PRO:HB2	1:B:216:TRP:CG	2.54	0.42
1:B:237:ASN:ND2	1:B:243:VAL:HG22	2.35	0.42
1:B:72:ASN:HD22	1:B:73:PRO:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LEU:HA	1:B:199:LEU:HD12	1.73	0.42
1:B:349:THR:O	1:B:350:SER:CB	2.67	0.42
3:A:1001:298:H14B	3:A:1001:298:N10	2.33	0.42
1:A:153:ARG:HG2	1:A:154:GLN:N	2.35	0.42
1:A:228:ARG:HH21	1:A:232:LYS:CA	2.33	0.42
1:B:361:VAL:HB	1:B:373:MET:HB3	2.02	0.42
2:A:801:FAD:C4X	3:A:1001:298:H9A	2.50	0.41
1:A:388:ARG:HH11	1:A:388:ARG:CB	2.33	0.41
1:B:461:ASP:HB2	4:B:1086:HOH:O	2.19	0.41
1:B:63:ALA:HA	2:B:802:FAD:C4X	2.50	0.41
1:B:240:ASP:OD1	1:B:241:GLY:N	2.52	0.41
1:A:388:ARG:NH1	1:A:438:SER:O	2.54	0.41
1:A:239:GLU:C	1:A:241:GLY:N	2.74	0.41
1:A:54:TYR:CD2	1:A:55:GLN:HG3	2.55	0.41
1:A:61:ILE:HA	1:A:61:ILE:HD12	1.94	0.41
1:B:219:LEU:O	1:B:220:SER:HB2	2.21	0.41
1:B:44:VAL:CG1	1:B:217:LEU:HD21	2.50	0.41
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.81	0.41
1:B:509:LEU:C	1:B:511:HIS:H	2.24	0.41
1:A:221:CYS:SG	1:A:221:CYS:O	2.79	0.41
1:B:143:GLN:O	1:B:147:LYS:HG3	2.21	0.41
1:A:122:MET:O	1:A:125:PHE:HB3	2.21	0.40
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.92	0.40
1:B:99:TYR:O	1:B:106:ARG:HA	2.21	0.40
1:B:451:SER:O	3:B:1002:298:H1B	2.20	0.40
1:B:250:ILE:HD11	1:B:503:ILE:HD12	2.02	0.40
1:A:401:VAL:O	1:A:405:ILE:HG13	2.21	0.40
1:A:147:LYS:HE2	1:A:151:GLN:NE2	2.37	0.40
1:A:359:PHE:O	1:A:374:MET:HA	2.21	0.40

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	491/516 (95%)	462 (94%)	26 (5%)	3 (1%)	28	29
1	B	490/516 (95%)	448 (91%)	35 (7%)	7 (1%)	13	10
All	All	981/1032 (95%)	910 (93%)	61 (6%)	10 (1%)	18	16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	265	GLU
1	B	200	ASN
1	B	136	VAL
1	B	137	SER
1	B	265	GLU
1	B	266	LYS
1	B	427	ALA
1	B	421	ILE
1	A	230	PRO

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	414/457 (91%)	401 (97%)	13 (3%)	45	57
1	B	405/457 (89%)	391 (96%)	14 (4%)	41	51
All	All	819/914 (90%)	792 (97%)	27 (3%)	43	54

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	64	SER
1	A	139	CYS
1	A	177	LEU
1	A	179	TRP
1	A	201	TYR

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Mol	Chain	Res	Type
1	A	218	LYS
1	A	221	CYS
1	A	267	ASN
1	A	291	PHE
1	A	377	GLN
1	A	389	GLU
1	A	483	MET
1	B	64	SER
1	B	72	ASN
1	B	124	LYS
1	B	179	TRP
1	B	199	LEU
1	B	201	TYR
1	B	221	CYS
1	B	271	ARG
1	B	291	PHE
1	B	312	LYS
1	B	336	LEU
1	B	377	GLN
1	B	380	LEU
1	B	412	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	33	GLN
1	A	151	GLN
1	A	158	ASN
1	A	267	ASN
1	A	332	ASN
1	A	362	ASN
1	A	377	GLN
1	A	434	ASN
1	B	29	GLN
1	B	72	ASN
1	B	237	ASN
1	B	267	ASN
1	B	290	HIS
1	B	329	ASN
1	B	362	ASN
1	B	377	GLN

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Mol	Chain	Res	Type
1	B	434	ASN
1	B	439	ASN

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 ⓘ

4 ligands 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
3	298	A	1001	-	13,13,13	1.83	4 (30%)	10,12,12	1.94	4 (40%)
2	FAD	A	801	-	51,58,58	1.51	9 (17%)	54,89,89	2.60	14 (25%)
3	298	B	1002	-	13,13,13	1.81	4 (30%)	10,12,12	2.03	4 (40%)
2	FAD	B	802	-	51,58,58	1.50	8 (15%)	54,89,89	2.62	11 (20%)

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	298	A	1001	-	-	2/9/11/11	0/0/0/0
2	FAD	A	801	-	-	0/28/50/50	0/6/6/6
3	298	B	1002	-	-	0/9/11/11	0/0/0/0
2	FAD	B	802	-	-	0/28/50/50	0/6/6/6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	298	C14-C13	-2.42	1.39	1.49
3	B	1002	298	C14-C13	-2.41	1.39	1.49
3	B	1002	298	C1-C2	-2.40	1.39	1.49
3	A	1001	298	C1-C2	-2.38	1.39	1.49
2	B	802	FAD	C5X-N5	2.09	1.38	1.35
2	B	802	FAD	C5B-C4B	2.18	1.58	1.51
2	A	801	FAD	C2A-N1A	2.26	1.38	1.33
2	A	801	FAD	O4B-C1B	2.26	1.44	1.41
2	A	801	FAD	C2A-N3A	2.36	1.36	1.32
2	B	802	FAD	C2A-N3A	2.37	1.36	1.32
2	A	801	FAD	C5B-C4B	2.44	1.59	1.51
2	B	802	FAD	C2A-N1A	2.47	1.38	1.33
2	A	801	FAD	C5X-N5	2.60	1.39	1.35
2	B	802	FAD	C4-N3	3.14	1.38	1.33
2	A	801	FAD	C9A-N10	3.20	1.42	1.38
2	A	801	FAD	C4-N3	3.42	1.39	1.33
3	B	1002	298	C3-C2	3.47	1.39	1.32
3	B	1002	298	C12-C13	3.48	1.39	1.32
3	A	1001	298	C3-C2	3.48	1.39	1.32
2	A	801	FAD	C10-N1	3.50	1.38	1.33
3	A	1001	298	C12-C13	3.59	1.39	1.32
2	B	802	FAD	C10-N1	3.64	1.38	1.33
2	B	802	FAD	C4X-N5	4.20	1.39	1.33
2	B	802	FAD	C9A-N10	4.34	1.44	1.38
2	A	801	FAD	C4X-N5	4.73	1.40	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	O2A-PA-O5B	-8.00	70.39	108.14
2	B	802	FAD	O2A-PA-O5B	-7.51	72.67	108.14
2	A	801	FAD	O2A-PA-O1A	-5.76	82.48	112.28
2	B	802	FAD	O2A-PA-O1A	-5.57	83.43	112.28
2	B	802	FAD	C4X-C4-N3	-4.54	117.03	123.48
2	A	801	FAD	C4X-C4-N3	-4.22	117.48	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	FAD	N3A-C2A-N1A	-4.09	125.30	128.86
2	A	801	FAD	N3A-C2A-N1A	-3.96	125.41	128.86
3	A	1001	298	C9-N10-C11	-3.30	109.70	118.38
3	A	1001	298	C6-N5-C4	-3.14	110.12	118.38
3	B	1002	298	C6-N5-C4	-3.14	110.14	118.38
3	B	1002	298	C1-C2-C3	-3.12	119.88	125.74
3	A	1001	298	C1-C2-C3	-3.11	119.90	125.74
3	B	1002	298	C9-N10-C11	-2.95	110.62	118.38
3	B	1002	298	C14-C13-C12	-2.86	120.37	125.74
2	B	802	FAD	C4B-O4B-C1B	-2.78	106.81	109.77
2	B	802	FAD	O3'-C3'-C4'	-2.51	102.60	108.82
2	A	801	FAD	C4-C4X-C10	-2.36	118.06	119.96
2	A	801	FAD	O3'-C3'-C4'	-2.31	103.08	108.82
3	A	1001	298	C14-C13-C12	-2.30	121.42	125.74
2	A	801	FAD	C4B-O4B-C1B	-2.13	107.50	109.77
2	B	802	FAD	C4X-C10-N10	-2.09	119.07	120.52
2	A	801	FAD	C4X-C10-N10	-2.04	119.10	120.52
2	A	801	FAD	C4-C4X-N5	2.13	121.01	118.68
2	A	801	FAD	C5X-C9A-N10	2.14	119.25	117.66
2	A	801	FAD	C1'-N10-C9A	3.01	121.11	118.35
2	A	801	FAD	C4X-N5-C5X	3.69	120.66	116.76
2	B	802	FAD	C1'-N10-C9A	3.89	121.91	118.35
2	B	802	FAD	C4X-N5-C5X	4.28	121.28	116.76
2	B	802	FAD	O5B-PA-O1A	6.40	135.08	109.25
2	A	801	FAD	O5B-PA-O1A	7.01	137.52	109.25
2	A	801	FAD	C4-N3-C2	10.36	124.22	115.16
2	B	802	FAD	C4-N3-C2	10.55	124.38	115.16

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	298	C13-C12-C11-N10
3	A	1001	298	C2-C3-C4-N5

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	298	8	0
2	A	801	FAD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	298	2	0
2	B	802	FAD	2	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, 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	497/516 (96%)	0.08	25 (5%)	30 28	21, 37, 61, 85	0
1	B	496/516 (96%)	0.32	36 (7%)	16 15	29, 42, 68, 81	0
All	All	993/1032 (96%)	0.20	61 (6%)	22 21	21, 39, 65, 85	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	342	ARG	6.8
1	B	136	VAL	6.3
1	B	511	HIS	5.0
1	A	230	PRO	4.7
1	B	425	ALA	4.3
1	B	135	GLY	4.3
1	A	231	SER	4.3
1	A	343	GLU	4.2
1	B	230	PRO	4.2
1	B	137	SER	3.9
1	A	131	HIS	3.6
1	A	5	SER	3.5
1	B	264	PRO	3.5
1	B	267	ASN	3.4
1	B	289	ILE	3.4
1	B	266	LYS	3.3
1	B	339	MET	3.3
1	A	14	ILE	3.3
1	A	133	HIS	3.3
1	B	231	SER	3.3
1	A	253	VAL	3.1
1	A	350	SER	3.1
1	A	251	ILE	3.0
1	A	264	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	342	ARG	2.9
1	B	252	THR	2.8
1	B	250	ILE	2.8
1	A	427	ALA	2.7
1	B	14	ILE	2.7
1	A	428	ASN	2.7
1	A	238	CYS	2.6
1	B	131	HIS	2.6
1	B	245	ASN	2.6
1	B	338	SER	2.6
1	B	251	ILE	2.6
1	B	340	LEU	2.5
1	A	168	CYS	2.4
1	B	33	GLN	2.4
1	B	361	VAL	2.4
1	B	173	LEU	2.4
1	B	420	PRO	2.4
1	B	84	ASN	2.4
1	B	13	ILE	2.3
1	A	232	LYS	2.3
1	A	511	HIS	2.3
1	B	458	ASP	2.3
1	A	252	THR	2.2
1	A	339	MET	2.2
1	A	136	VAL	2.2
1	B	421	ILE	2.2
1	A	6	PRO	2.2
1	B	423	ASN	2.2
1	B	38	LEU	2.1
1	A	221	CYS	2.1
1	B	374	MET	2.1
1	B	138	ASP	2.1
1	B	265	GLU	2.1
1	B	454	PHE	2.1
1	A	13	ILE	2.0
1	B	359	PHE	2.0
1	A	340	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	298	A	1001	14/14	0.75	0.35	4.41	58,62,68,69	0
3	298	B	1002	14/14	0.75	0.35	3.90	60,62,63,63	0
2	FAD	B	802	53/53	0.92	0.20	0.51	30,38,42,49	0
2	FAD	A	801	53/53	0.95	0.19	0.46	18,27,33,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.