Full wwPDB X-ray Structure Validation Report (i)

PDB ID : 3ZNP
Title : IN VITRO AND IN VIVO INHIBITION OF HUMAN D-AMINO ACID OXI-
DASE: REGULATION OF D-SERINE CONCENTRATION IN THE BRAIN
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Hardy, L.W.; Orsini, M.A.; Allen, M.S.; Koch, P.; Spear, K.L.; Foglesong, R.J.;
Soukri, M.; Chytil, M.; Fang, Q.K.; Jones, S.W.; Varney, M.A.; Panatier, A.;
Oliet, S.H.R.; Pollegioni, L.; Piubelli, L.; Molla, G.; Nardini, M.; Large, T.H.
Deposited on : 2013-02-15
Resolution : 2.40 Å(reported)

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	Percentile Ranks	Value
Rfree		0.310
Clashscore		5
Ramachandran outliers		0.7%
Sidechain outliers		9.4%
RSRZ outliers		21.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
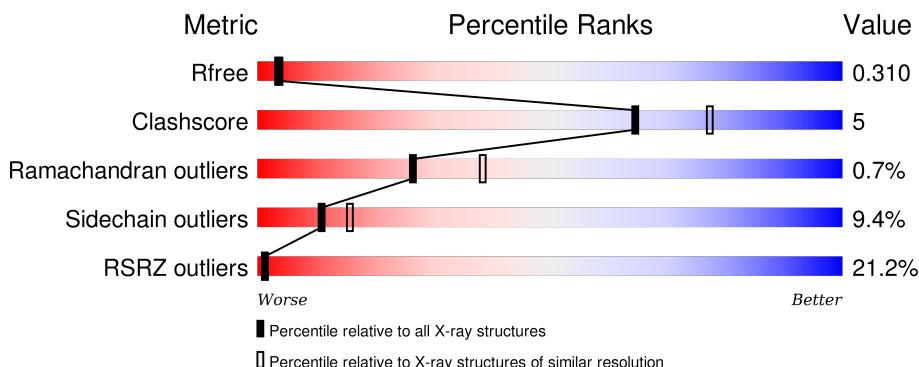
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	12% / 81% 15% · ·
1	B	347	30% / 77% 19% · ·
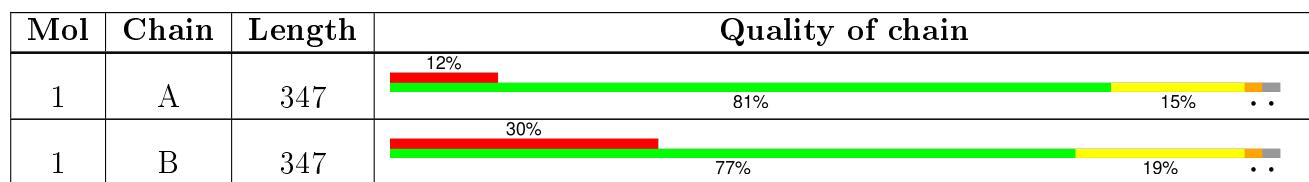
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SE2	A	360	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5815 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 D-AMINO-ACID OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total 2786	C 1787	N 495	O 495	S 9	0	7	0
1	B	340	Total 2754	C 1766	N 485	O 494	S 9	0	3	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
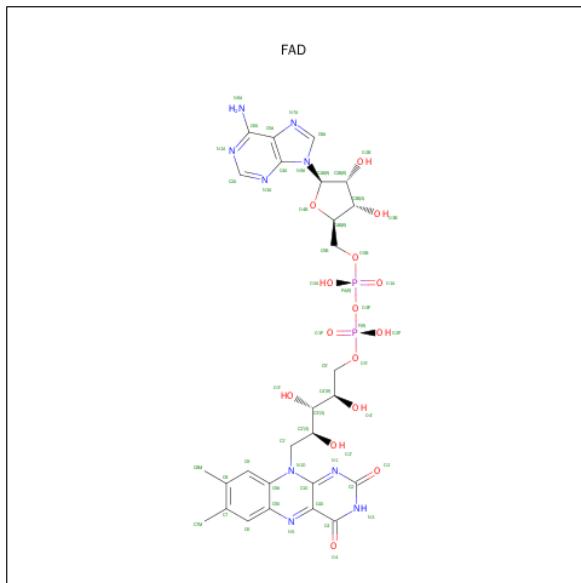
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is 3-HYDROXY-2H-CHROMEN-2-ONE (three-letter code: SE2) (formula: $C_9H_6O_3$).

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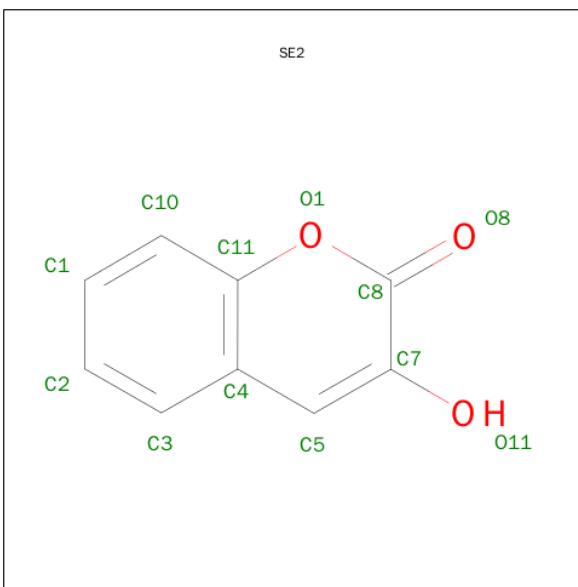
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	9	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	1
			12	6	6		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total 79	O 79	0	9
5	B	29	Total 30	O 30	0	1

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: D-AMINO-ACID OXIDASE
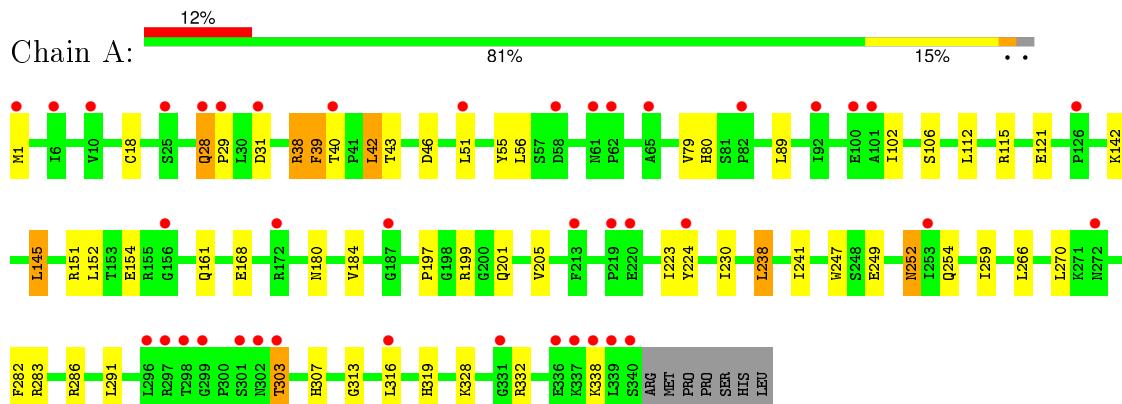
- Molecule 1: D-AMINO-ACID OXIDASE
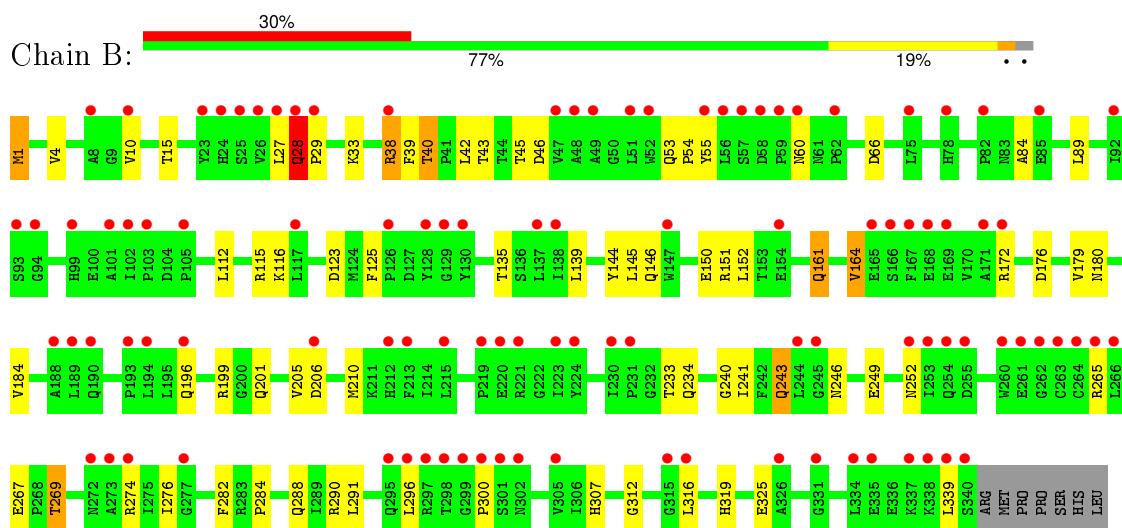
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	84.07Å 84.07Å 189.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.98 – 2.40 34.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.98-2.40) 98.2 (34.98-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.232 , 0.307 0.233 , 0.310	Depositor DCC
R_{free} test set	1539 reflections (5.31%)	DCC
Wilson B-factor (Å²)	57.3	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 72.1	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \lvert L \rvert > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 30523 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5815	wwPDB-VP
Average B, all atoms (Å²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, SE2, 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	0.51	0/2882	0.78	4/3917 (0.1%)
1	B	0.48	0/2840	0.73	0/3863
All	All	0.50	0/5722	0.76	4/7780 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	303	THR	N-CA-C	9.68	137.15	111.00
1	A	39	PHE	C-N-CA	6.90	138.95	121.70
1	A	39	PHE	CB-CA-C	6.67	123.75	110.40
1	A	303	THR	CB-CA-C	-5.17	97.64	111.60

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	2786	0	2762	29	0
1	B	2754	0	2717	33	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
3	A	12	0	5	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	30	0	40	0	0
4	B	18	0	24	0	0
5	A	79	0	0	0	0
5	B	30	0	0	0	0
All	All	5815	0	5610	58	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 5.

All (58) 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:303:THR:O	1:A:303:THR:HG22	1.74	0.87
1:A:180:ASN:HD22	1:A:307:HIS:HD2	1.25	0.82
1:A:39:PHE:O	1:A:43:THR:HG23	1.81	0.81
1:A:51:LEU:HD23	3:A:360:SE2:H1	1.66	0.78
1:B:28:GLN:HB2	1:B:29:PRO:HD3	1.74	0.69
1:A:313:GLY:O	3:A:360:SE2:H5	1.93	0.67
1:A:38[A]:ARG:HG2	2:A:350:FAD:O2B	1.95	0.64
1:A:79:VAL:HG13	1:A:80:HIS:HD2	1.64	0.63
1:A:161:GLN:HE21	1:B:249:GLU:H	1.46	0.63
1:A:316:LEU:O	1:A:319:HIS:HD2	1.82	0.63
1:A:230:ILE:HD11	3:A:360:SE2:H10	1.81	0.62
1:B:164:VAL:HG23	2:B:350:FAD:N1A	2.15	0.61
1:A:28:GLN:HG2	1:A:29:PRO:HD3	1.84	0.60
1:A:40:THR:O	1:A:46:ASP:OD1	2.20	0.59
1:A:201:GLN:HE22	1:A:252:ASN:H	1.50	0.59
1:B:233:THR:HG23	1:B:234:GLN:HG2	1.85	0.58
1:B:201:GLN:HE22	1:B:252:ASN:H	1.51	0.58
1:A:180:ASN:HD22	1:A:307:HIS:CD2	2.15	0.57
1:B:206:ASP:HB3	1:B:274:ARG:HG3	1.87	0.57
1:A:328:LYS:HE2	1:A:332:ARG:HH12	1.70	0.56
1:B:15:THR:HG21	1:B:179:VAL:HG11	1.87	0.56
1:B:112:LEU:HB2	1:B:135:THR:HB	1.89	0.55
1:B:199:ARG:HH22	1:B:201:GLN:HE21	1.54	0.54
1:B:199:ARG:HH22	1:B:201:GLN:NE2	2.07	0.52
1:B:316:LEU:O	1:B:319:HIS:HD2	1.93	0.52
1:A:199:ARG:HH22	1:A:201:GLN:HE21	1.59	0.51
1:B:40:THR:O	1:B:46:ASP:OD1	2.29	0.51
1:A:241:ILE:HD13	1:A:259:ILE:HG13	1.93	0.50
1:B:243:GLN:HE21	1:B:246:ASN:HD22	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLU:H	1:B:161:GLN:HE21	1.60	0.50
1:A:55:TYR:HE1	1:A:224:TYR:HH	1.59	0.49
1:B:284:PRO:HD2	1:B:312:GLY:O	2.13	0.49
1:A:161:GLN:NE2	1:B:249:GLU:H	2.11	0.48
1:B:267:GLU:HG3	1:B:269:THR:HG23	1.96	0.48
1:A:115:ARG:NH2	1:A:121:GLU:OE2	2.46	0.48
1:B:291:LEU:HD21	1:B:325:GLU:HB3	1.96	0.48
1:A:283:ARG:NE	3:A:360:SE2:O11	2.33	0.48
1:A:184:VAL:HG11	1:A:282:PHE:HB2	1.95	0.48
1:B:38[A]:ARG:HG2	2:B:350:FAD:O2B	2.15	0.47
1:B:39:PHE:O	1:B:43:THR:HG23	2.16	0.46
1:A:40:THR:HG23	1:A:145:LEU:HB3	1.97	0.45
1:B:1:MET:HA	1:B:176:ASP:OD2	2.16	0.45
1:B:144:TYR:OH	1:B:319:HIS:CE1	2.70	0.45
1:B:144:TYR:OH	1:B:319:HIS:HE1	1.99	0.45
1:A:197:PRO:HG3	1:A:247:TRP:CE2	2.52	0.44
1:B:10:VAL:HB	1:B:45:THR:HG21	1.98	0.44
1:B:139:LEU:HD11	1:B:144:TYR:CD1	2.53	0.43
1:B:53:GLN:HA	1:B:54:PRO:HD3	1.89	0.43
1:B:4:VAL:HG22	1:B:33:LYS:HB2	2.01	0.43
1:B:184:VAL:HG11	1:B:282:PHE:HB2	2.00	0.42
1:B:180:ASN:HB3	1:B:307:HIS:HA	2.02	0.42
1:A:180:ASN:ND2	1:A:307:HIS:HD2	2.04	0.42
1:B:146:GLN:HE21	1:B:150:GLU:HG3	1.84	0.42
1:A:291:LEU:HA	1:A:307:HIS:O	2.20	0.41
1:B:201:GLN:NE2	1:B:252:ASN:H	2.16	0.41
1:A:42:LEU:HD22	1:B:42:LEU:HD23	2.03	0.41
1:B:180:ASN:HD22	1:B:307:HIS:HD2	1.69	0.40
1:A:238:LEU:HD11	1:A:270:LEU:HD21	2.03	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	345/347 (99%)	324 (94%)	21 (6%)	0	100	100
1	B	341/347 (98%)	306 (90%)	30 (9%)	5 (2%)	13	17
All	All	686/694 (99%)	630 (92%)	51 (7%)	5 (1%)	26	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	PRO
1	B	40	THR
1	B	28	GLN
1	B	84	ALA
1	B	240	GLY

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	299/299 (100%)	273 (91%)	26 (9%)	13	19
1	B	295/299 (99%)	264 (90%)	31 (10%)	8	12
All	All	594/598 (99%)	537 (90%)	57 (10%)	11	15

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	CYS
1	A	28	GLN
1	A	31	ASP
1	A	38[A]	ARG
1	A	38[B]	ARG
1	A	42	LEU
1	A	56	LEU
1	A	89	LEU
1	A	102	ILE
1	A	106	SER

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Mol	Chain	Res	Type
1	A	112	LEU
1	A	142	LYS
1	A	145	LEU
1	A	151	ARG
1	A	152	LEU
1	A	154	GLU
1	A	168	GLU
1	A	205	VAL
1	A	223	ILE
1	A	238	LEU
1	A	252	ASN
1	A	254	GLN
1	A	266	LEU
1	A	286	ARG
1	A	338	LYS
1	B	1	MET
1	B	27	LEU
1	B	28	GLN
1	B	38[A]	ARG
1	B	38[B]	ARG
1	B	55	TYR
1	B	60	ASN
1	B	66	ASP
1	B	89	LEU
1	B	115	ARG
1	B	116	LYS
1	B	123	ASP
1	B	125	PHE
1	B	145	LEU
1	B	151	ARG
1	B	152	LEU
1	B	161	GLN
1	B	164	VAL
1	B	172	ARG
1	B	196	GLN
1	B	205	VAL
1	B	210	MET
1	B	241	ILE
1	B	243	GLN
1	B	265	ARG
1	B	269	THR
1	B	276	ILE

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Mol	Chain	Res	Type
1	B	288	GLN
1	B	290	ARG
1	B	296	LEU
1	B	339	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	161	GLN
1	A	201	GLN
1	A	243	GLN
1	A	252	ASN
1	A	307	HIS
1	A	319	HIS
1	B	28	GLN
1	B	53	GLN
1	B	80	HIS
1	B	96	ASN
1	B	146	GLN
1	B	161	GLN
1	B	180	ASN
1	B	196	GLN
1	B	201	GLN
1	B	243	GLN
1	B	252	ASN
1	B	307	HIS
1	B	319	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)

11 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	#$|Z| > 2$
4	GOL	A	1341	-	5,5,5	0.66	0	5,5,5	0.67	0
4	GOL	A	1342[A]	-	5,5,5	0.34	0	5,5,5	0.23	0
4	GOL	A	1342[B]	-	5,5,5	0.36	0	5,5,5	0.24	0
4	GOL	A	1343	-	5,5,5	0.81	0	5,5,5	0.72	0
4	GOL	A	1344	-	5,5,5	0.53	0	5,5,5	0.57	0
2	FAD	A	350	-	48,58,58	2.70	20 (41%)	54,89,89	3.83	21 (38%)
3	SE2	A	360	-	11,13,13	2.16	2 (18%)	12,18,18	1.93	3 (25%)
4	GOL	B	1341	-	5,5,5	0.65	0	5,5,5	0.55	0
4	GOL	B	1342	-	5,5,5	0.57	0	5,5,5	0.53	0
4	GOL	B	1343	-	5,5,5	0.60	0	5,5,5	0.52	0
2	FAD	B	350	-	48,58,58	2.66	14 (29%)	54,89,89	3.32	21 (38%)

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
4	GOL	A	1341	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1342[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1342[B]	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1343	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1344	-	-	0/4/4/4	0/0/0/0
2	FAD	A	350	-	-	0/30/50/50	0/6/6/6
3	SE2	A	360	-	-	0/0/0/0	0/2/2/2
4	GOL	B	1341	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1342	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1343	-	-	0/4/4/4	0/0/0/0
2	FAD	B	350	-	-	0/30/50/50	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	FAD	P-O1P	-4.60	1.34	1.51
2	A	350	FAD	C10-N10	-3.04	1.35	1.39
2	A	350	FAD	C1'-N10	-2.97	1.45	1.48
2	B	350	FAD	O4B-C4B	-2.87	1.38	1.45
2	B	350	FAD	C10-N10	-2.48	1.36	1.39
2	B	350	FAD	P-O1P	-2.37	1.42	1.51
2	A	350	FAD	C2B-C3B	-2.32	1.47	1.53
2	A	350	FAD	O4B-C4B	-2.26	1.39	1.45
2	A	350	FAD	O3B-C3B	-2.19	1.37	1.43
3	A	360	SE2	C5-C7	2.11	1.39	1.37
2	A	350	FAD	C3B-C4B	2.11	1.58	1.53
2	A	350	FAD	C8A-N7A	2.31	1.39	1.34
2	B	350	FAD	C10-N1	2.40	1.39	1.35
2	A	350	FAD	C4-N3	2.52	1.37	1.33
2	A	350	FAD	C4'-C3'	2.53	1.58	1.53
2	B	350	FAD	C2A-N3A	2.68	1.36	1.32
2	B	350	FAD	C8A-N7A	2.73	1.39	1.34
2	A	350	FAD	C6-C5X	2.80	1.46	1.41
2	A	350	FAD	C9-C9A	2.84	1.46	1.40
2	B	350	FAD	C9-C9A	3.10	1.47	1.40
2	A	350	FAD	O4B-C1B	3.23	1.45	1.41
2	A	350	FAD	C10-N1	3.28	1.41	1.35
2	B	350	FAD	C4X-N5	3.37	1.38	1.33
2	B	350	FAD	O4-C4	3.73	1.33	1.24
2	B	350	FAD	C4-N3	3.90	1.40	1.33
2	B	350	FAD	C5X-N5	4.07	1.41	1.35
2	B	350	FAD	C6-C5X	4.21	1.48	1.41
2	A	350	FAD	C7M-C7	4.48	1.60	1.51
2	A	350	FAD	O4-C4	4.56	1.35	1.24
2	A	350	FAD	C4X-N5	4.74	1.40	1.33
2	A	350	FAD	C5X-N5	4.76	1.43	1.35
3	A	360	SE2	C4-C11	6.19	1.49	1.41
2	A	350	FAD	C4X-C10	7.54	1.55	1.41
2	B	350	FAD	C4X-C10	8.77	1.57	1.41
2	A	350	FAD	C9A-N10	8.85	1.51	1.38
2	B	350	FAD	C9A-N10	10.62	1.53	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	FAD	N3A-C2A-N1A	-19.74	113.78	128.89
2	B	350	FAD	N3A-C2A-N1A	-15.99	116.65	128.89
2	A	350	FAD	C4X-C10-N10	-7.66	116.01	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	FAD	C4-C4X-C10	-7.32	115.26	119.94
2	B	350	FAD	C4X-C10-N10	-7.00	116.39	120.52
2	B	350	FAD	C4-C4X-C10	-6.46	115.81	119.94
2	A	350	FAD	C4A-C5A-N7A	-5.82	104.12	109.48
2	B	350	FAD	C4A-C5A-N7A	-4.73	105.13	109.48
3	A	360	SE2	C10-C11-C4	-4.12	118.80	123.14
2	A	350	FAD	O4'-C4'-C5'	-3.61	102.32	110.19
2	A	350	FAD	O5B-C5B-C4B	-3.60	95.84	109.12
2	B	350	FAD	C9A-C5X-N5	-3.33	117.43	122.36
2	B	350	FAD	O5B-C5B-C4B	-3.23	97.20	109.12
2	A	350	FAD	C9A-C5X-N5	-3.10	117.77	122.36
2	B	350	FAD	C1B-N9A-C4A	-2.81	122.70	126.94
2	A	350	FAD	C9-C9A-C5X	-2.58	115.04	119.62
2	B	350	FAD	O2A-PA-O3P	-2.49	93.81	105.09
2	B	350	FAD	O3P-P-O5'	-2.45	96.45	102.94
2	A	350	FAD	C4B-O4B-C1B	-2.38	107.11	109.72
2	B	350	FAD	O3B-C3B-C4B	-2.37	103.95	111.05
2	A	350	FAD	O3P-P-O5'	-2.30	96.83	102.94
2	B	350	FAD	O2P-P-O5'	-2.28	96.97	108.46
2	B	350	FAD	C9-C9A-C5X	-2.06	115.95	119.62
2	A	350	FAD	O3B-C3B-C4B	-2.03	104.96	111.05
2	B	350	FAD	C2A-N1A-C6A	2.00	122.35	118.77
2	A	350	FAD	C2B-C3B-C4B	2.21	107.15	102.61
2	A	350	FAD	C1'-N10-C9A	2.31	121.46	118.86
2	B	350	FAD	O3'-C3'-C2'	2.42	114.86	108.75
3	A	360	SE2	C5-C4-C11	2.43	119.72	116.65
2	B	350	FAD	O4B-C1B-N9A	2.44	113.22	108.10
2	B	350	FAD	C4-N3-C2	2.45	117.36	115.25
2	A	350	FAD	O3'-C3'-C2'	2.67	115.47	108.75
2	A	350	FAD	C2A-N1A-C6A	2.93	124.00	118.77
2	B	350	FAD	C6-C5X-N5	2.95	122.76	118.96
2	A	350	FAD	C6-C5X-N5	3.37	123.30	118.96
2	A	350	FAD	C5X-C9A-N10	3.79	120.50	117.62
3	A	360	SE2	O1-C11-C10	4.04	121.12	116.10
2	B	350	FAD	O2P-P-O1P	4.23	135.45	112.53
2	A	350	FAD	O2P-P-O1P	4.37	136.21	112.53
2	B	350	FAD	C5X-C9A-N10	4.44	121.00	117.62
2	B	350	FAD	C4-C4X-N5	4.95	124.73	118.72
2	A	350	FAD	C4-C4X-N5	5.19	125.02	118.72
2	A	350	FAD	C4-N3-C2	5.39	119.91	115.25
2	A	350	FAD	C4X-N5-C5X	5.53	123.12	116.76
2	B	350	FAD	C4X-N5-C5X	6.72	124.49	116.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	FAD	1	0
3	A	360	SE2	4	0
2	B	350	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 (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, 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	340/347 (97%)	0.71	41 (12%)	6	5	31, 67, 140, 189	0
1	B	340/347 (97%)	1.63	103 (30%)	1	1	64, 96, 151, 192	0
All	All	680/694 (97%)	1.17	144 (21%)	1	1	31, 84, 148, 192	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	THR	9.3
1	A	297	ARG	9.2
1	B	26	VAL	7.9
1	B	299	GLY	7.4
1	B	25	SER	7.1
1	B	253	ILE	7.0
1	B	340	SER	7.0
1	B	339	LEU	6.9
1	B	56	LEU	6.9
1	B	223	ILE	6.8
1	A	298	THR	6.6
1	A	303	THR	6.2
1	B	57	SER	6.2
1	B	219	PRO	6.1
1	B	297	ARG	6.0
1	B	55	TYR	5.8
1	B	194	LEU	5.7
1	B	300	PRO	5.3
1	B	128	TYR	5.0
1	B	338	LYS	5.0
1	B	60	ASN	5.0
1	B	255	ASP	4.9
1	B	126	PRO	4.8
1	A	301	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	221	ARG	4.7
1	B	51	LEU	4.6
1	A	339	LEU	4.6
1	B	168	GLU	4.5
1	B	167	PHE	4.5
1	B	261	GLU	4.5
1	B	129	GLY	4.4
1	B	302	ASN	4.3
1	B	24	HIS	4.2
1	B	102	ILE	4.2
1	B	117	LEU	4.1
1	B	245	GLY	4.1
1	A	302	ASN	4.1
1	B	92	ILE	4.0
1	B	29	PRO	4.0
1	A	220	GLU	4.0
1	B	273	ALA	3.9
1	B	193	PRO	3.9
1	B	188	ALA	3.9
1	B	103	PRO	3.9
1	B	316	LEU	3.9
1	B	230	ILE	3.9
1	B	49	ALA	3.9
1	B	137	LEU	3.9
1	A	29	PRO	3.8
1	B	274	ARG	3.7
1	A	338	LYS	3.7
1	B	295	GLN	3.7
1	B	138[A]	ILE	3.7
1	A	337	LYS	3.7
1	B	172	ARG	3.6
1	B	166	SER	3.5
1	A	62	PRO	3.5
1	B	337	LYS	3.5
1	B	48	ALA	3.4
1	A	65	ALA	3.4
1	B	331	GLY	3.4
1	A	126	PRO	3.4
1	B	28	GLN	3.4
1	B	190	GLN	3.4
1	B	189	LEU	3.3
1	B	165	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	254	GLN	3.1
1	B	244	LEU	3.1
1	B	263	CYS	3.1
1	B	169	GLU	3.1
1	A	100	GLU	3.0
1	A	336	GLU	3.0
1	A	40	THR	3.0
1	B	212	HIS	3.0
1	B	220	GLU	3.0
1	B	27	LEU	2.9
1	A	253	ILE	2.9
1	B	296	LEU	2.9
1	A	316	LEU	2.8
1	B	266	LEU	2.8
1	B	38[A]	ARG	2.8
1	B	264	CYS	2.8
1	B	272	ASN	2.8
1	B	262	GLY	2.8
1	A	296	LEU	2.7
1	B	265	ARG	2.7
1	A	25	SER	2.7
1	B	260	TRP	2.7
1	B	101	ALA	2.7
1	A	172[A]	ARG	2.6
1	B	52	TRP	2.6
1	B	10	VAL	2.6
1	B	305	VAL	2.6
1	B	315	GLY	2.5
1	B	252	ASN	2.5
1	A	219	PRO	2.5
1	A	272	ASN	2.5
1	B	147	TRP	2.5
1	A	51	LEU	2.4
1	B	196	GLN	2.4
1	A	299	GLY	2.4
1	A	1	MET	2.4
1	A	28	GLN	2.4
1	B	326	ALA	2.4
1	B	130	TYR	2.4
1	A	82	PRO	2.4
1	B	78	HIS	2.4
1	A	331	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	224	TYR	2.4
1	A	10	VAL	2.4
1	A	6	ILE	2.3
1	B	215	LEU	2.3
1	A	340	SER	2.3
1	B	58	ASP	2.3
1	B	213	PHE	2.3
1	B	171	ALA	2.3
1	B	301	SER	2.3
1	B	334	LEU	2.3
1	A	224	TYR	2.3
1	B	23	TYR	2.3
1	A	101	ALA	2.2
1	B	99	HIS	2.2
1	B	154	GLU	2.2
1	B	59	PRO	2.2
1	A	213	PHE	2.2
1	B	335	GLU	2.2
1	B	75	LEU	2.2
1	B	62	PRO	2.2
1	B	277	GLY	2.2
1	B	47	VAL	2.1
1	B	8	ALA	2.1
1	B	93	SER	2.1
1	A	187	GLY	2.1
1	A	92	ILE	2.1
1	A	156	GLY	2.1
1	B	94	GLY	2.1
1	B	82	PRO	2.1
1	B	85	GLU	2.1
1	B	105	PRO	2.1
1	B	206	ASP	2.1
1	B	231	PRO	2.0
1	A	58	ASP	2.0
1	A	31	ASP	2.0
1	A	61	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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($Å^2$)	Q<0.9
4	GOL	B	1342	6/6	0.31	0.31	0.72	121,122,122,122	0
4	GOL	A	1344	6/6	0.75	0.24	0.37	96,98,98,98	0
2	FAD	B	350	53/53	0.88	0.19	-0.52	65,72,78,81	0
2	FAD	A	350	53/53	0.97	0.18	-0.55	32,44,61,67	0
3	SE2	A	360	12/12	0.91	0.20	-0.57	59,67,72,73	0
4	GOL	B	1343	6/6	0.19	0.46	-	116,117,117,118	0
4	GOL	A	1341	6/6	0.84	0.44	-	100,102,102,102	0
4	GOL	A	1343	6/6	0.38	0.55	-	102,104,104,104	0
4	GOL	A	1342[B]	6/6	0.78	0.28	-	103,104,104,105	6
4	GOL	B	1341	6/6	0.51	0.45	-	119,120,120,121	0
4	GOL	A	1342[A]	6/6	0.78	0.28	-	99,99,99,100	6

6.5 Other polymers (i)

There are no such residues in this entry.