



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:04 am GMT

PDB ID : 4YRW
Title : rat xanthine oxidoreductase, C-terminal deletion protein variant
Authors : Okamoto, K.
Deposited on : 2015-03-16
Resolution : 1.99 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

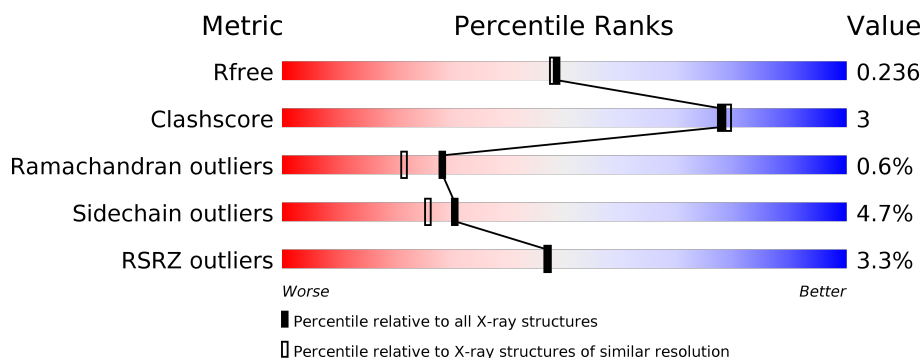
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	1315	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>...</div> </div> </div>
1	B	1315	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>9%</div> <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
6	URC	A	3006	-	X	-	-
6	URC	B	4006	-	X	-	-

2 Entry composition [i](#)

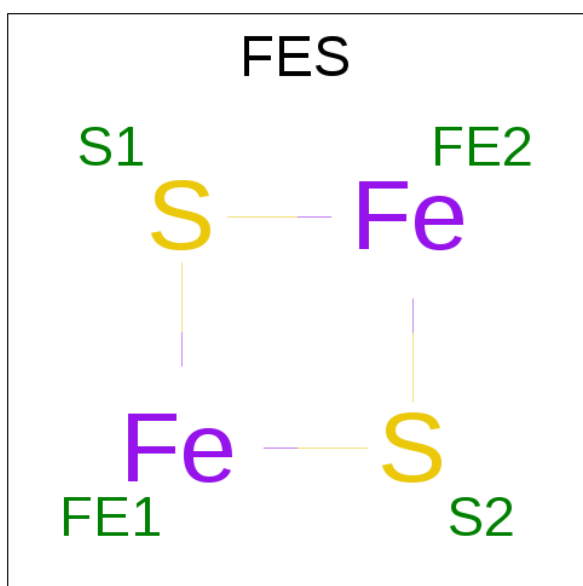
There are 8 unique types of molecules in this entry. The entry contains 20715 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Xanthine dehydrogenase/oxidase.

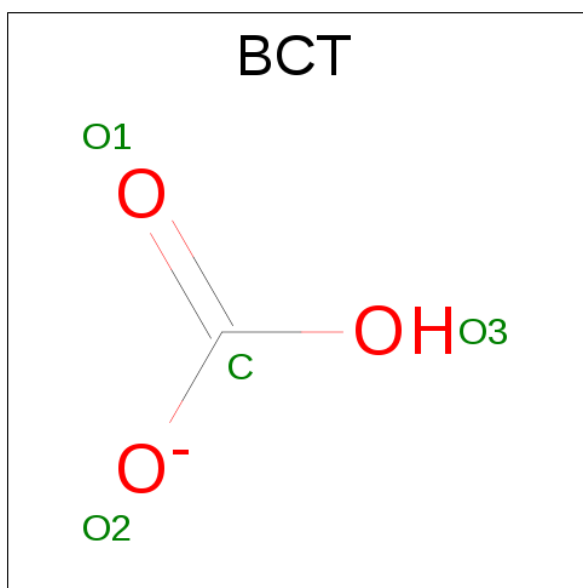
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1289	Total	C	N	O	S	0	0	0
			9964	6314	1714	1873	63			
1	B	1286	Total	C	N	O	S	0	0	0
			9939	6298	1711	1867	63			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

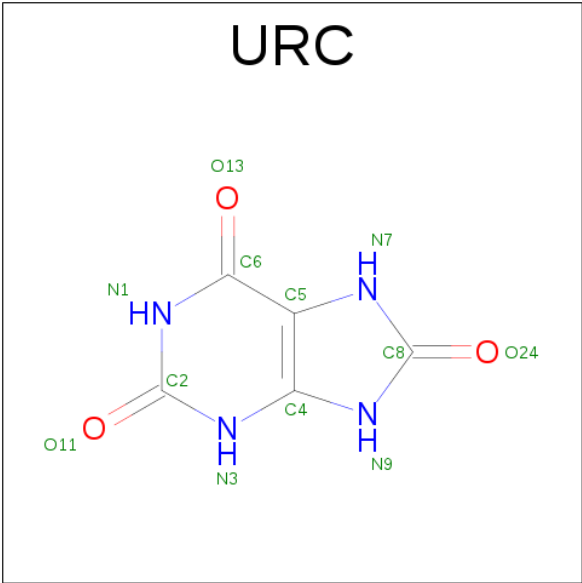
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



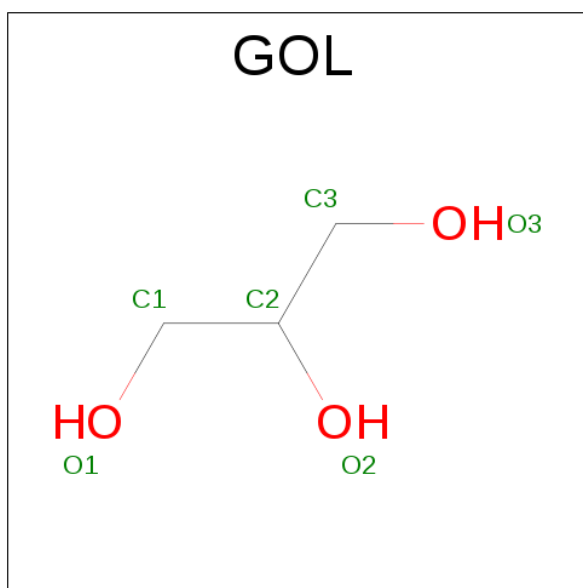
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is URIC ACID (three-letter code: URC) (formula: C₅H₄N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	5	4	3		
6	B	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

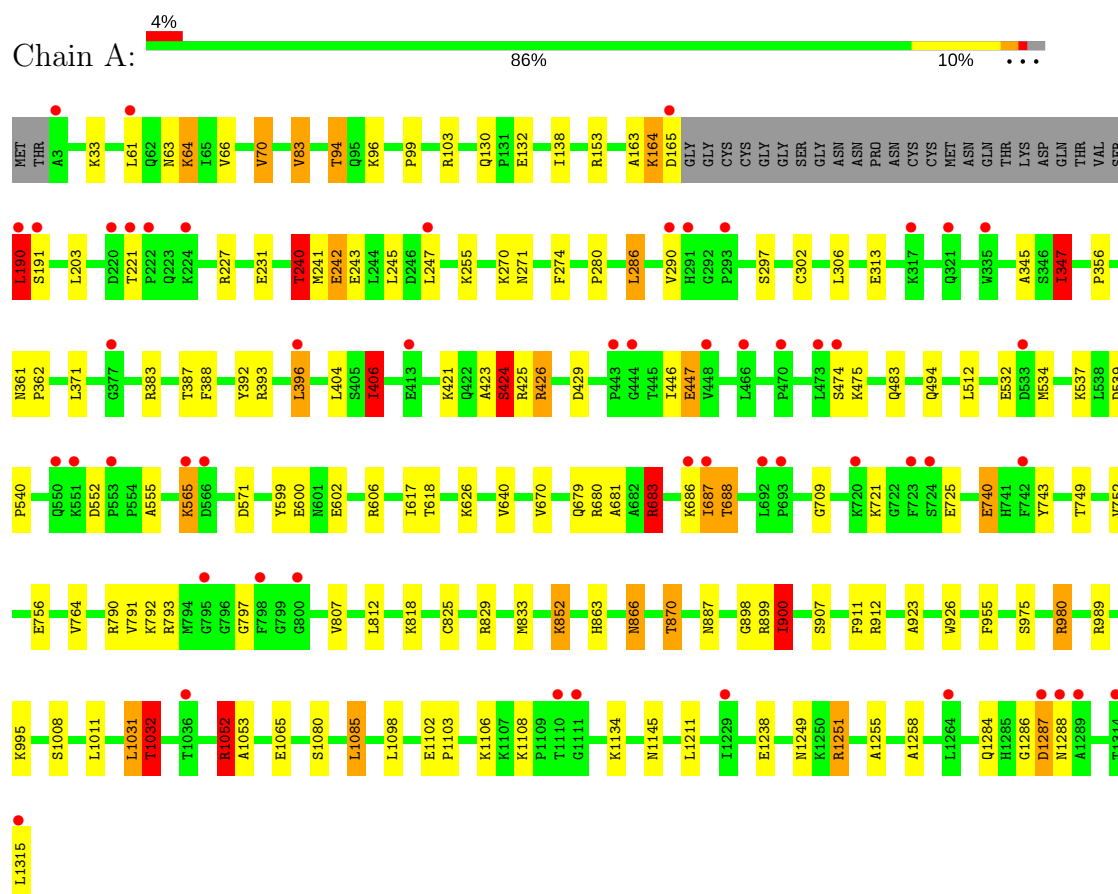
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	250	Total	O	0	0
			250	250		
8	B	388	Total	O	0	0
			388	388		

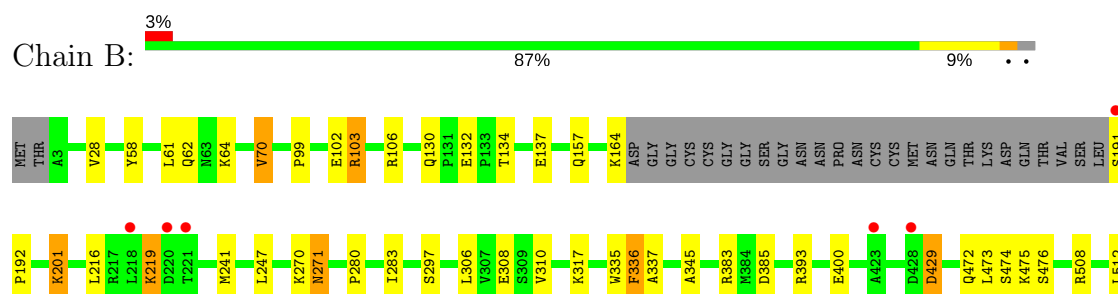
3 Residue-property plots

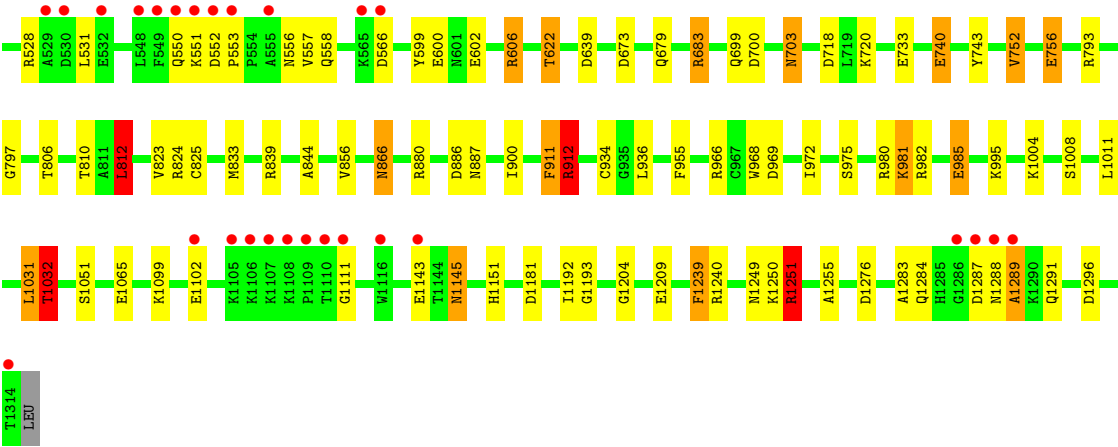
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Xanthine dehydrogenase/oxidase



• Molecule 1: Xanthine dehydrogenase/oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.50Å 138.47Å 222.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.33 – 1.99 43.33 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.33-1.99) 99.6 (43.33-1.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.229 0.194 , 0.236	Depositor DCC
R_{free} test set	10396 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.2	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	20715	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: GOL, URC, CA, FES, BCT, 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	0.94	4/10174 (0.0%)	1.00	28/13767 (0.2%)
1	B	1.06	12/10149 (0.1%)	1.04	44/13734 (0.3%)
All	All	1.00	16/20323 (0.1%)	1.02	72/27501 (0.3%)

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	B	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	740	GLU	CD-OE1	9.56	1.36	1.25
1	B	740	GLU	CD-OE2	8.97	1.35	1.25
1	B	308	GLU	CD-OE2	-7.06	1.17	1.25
1	A	600	GLU	CD-OE2	5.94	1.32	1.25
1	B	756	GLU	CB-CG	-5.89	1.41	1.52
1	B	602	GLU	CD-OE1	5.84	1.32	1.25
1	B	1193	GLY	N-CA	5.53	1.54	1.46
1	A	602	GLU	CD-OE1	5.50	1.31	1.25
1	B	600	GLU	CD-OE2	5.47	1.31	1.25
1	B	793	ARG	CZ-NH1	5.34	1.40	1.33
1	B	1239	PHE	CG-CD2	5.28	1.46	1.38
1	A	240	THR	CB-CG2	-5.28	1.34	1.52
1	B	102	GLU	CD-OE2	-5.24	1.19	1.25
1	B	756	GLU	CD-OE1	5.19	1.31	1.25
1	A	740	GLU	CD-OE1	5.12	1.31	1.25
1	B	429	ASP	CB-CG	-5.11	1.41	1.51

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1052	ARG	NE-CZ-NH2	-14.64	112.98	120.30
1	B	812	LEU	CA-CB-CG	-13.46	84.34	115.30
1	A	1052	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	B	793	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	A	989	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	793	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	793	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	70	VAL	CG1-CB-CG2	7.80	123.38	110.90
1	B	1031	LEU	CB-CG-CD2	7.55	123.83	111.00
1	B	1251	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	70	VAL	CG1-CB-CG2	7.06	122.19	110.90
1	A	790	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	683	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	856	VAL	CG1-CB-CG2	6.72	121.66	110.90
1	B	385	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	703	ASN	N-CA-CB	-6.61	98.70	110.60
1	A	406	ILE	CB-CA-C	-6.47	98.66	111.60
1	B	508	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	839	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	B	1251	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	1111	GLY	N-CA-C	-6.28	97.39	113.10
1	A	227	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	201	LYS	CA-CB-CG	6.25	127.16	113.40
1	A	900	ILE	CB-CA-C	6.23	124.05	111.60
1	B	1296	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	829	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	1032	THR	CB-CA-C	-6.15	94.99	111.60
1	B	740	GLU	OE1-CD-OE2	6.13	130.65	123.30
1	B	103	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	980	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	880	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	812	LEU	CD1-CG-CD2	6.07	128.70	110.50
1	B	912	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	83	VAL	CG1-CB-CG2	6.03	120.55	110.90
1	B	297	SER	CB-CA-C	6.00	121.50	110.10
1	B	793	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	1032	THR	N-CA-CB	5.93	121.57	110.30
1	B	1032	THR	CB-CA-C	-5.93	95.60	111.60
1	A	606	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	B	106	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	227	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	B	752	VAL	CG1-CB-CG2	5.85	120.25	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	LEU	CB-CG-CD1	5.83	120.91	111.00
1	B	639	ASP	CB-CG-OD2	5.82	123.53	118.30
1	B	880	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	1004	LYS	CD-CE-NZ	5.77	124.97	111.70
1	B	756	GLU	CB-CA-C	-5.73	98.93	110.40
1	B	718	ASP	CB-CG-OD1	5.68	123.42	118.30
1	B	385	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	393	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	824	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	673	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	1085	LEU	CB-CG-CD1	5.50	120.35	111.00
1	B	528	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	347	ILE	CB-CA-C	-5.43	100.74	111.60
1	A	203	LEU	CA-CB-CG	5.43	127.78	115.30
1	B	429	ASP	N-CA-CB	-5.42	100.84	110.60
1	A	683	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	966	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	606	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	622	THR	N-CA-CB	-5.30	100.23	110.30
1	A	1031	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	989	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	1032	THR	OG1-CB-CG2	5.22	122.02	110.00
1	A	94	THR	N-CA-CB	-5.18	100.45	110.30
1	B	508	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	1296	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	1251	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	756	GLU	CG-CD-OE2	-5.09	108.12	118.30
1	B	1276	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	B	1181	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	B	700	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	886	ASP	Peptide

5.2 Too-close contacts

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	9964	0	9967	78	0
1	B	9939	0	9942	59	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	53	0	31	1	0
5	B	53	0	31	2	0
6	A	12	0	4	0	0
6	B	12	0	4	0	0
7	A	6	0	8	0	0
7	B	12	0	16	0	0
8	A	250	0	0	1	0
8	B	388	0	0	5	0
All	All	20715	0	20003	135	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 3.

All (135) 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:982:ARG:NH1	8:B:4101:HOH:O	1.56	1.21
1:B:192:PRO:HD2	8:B:4376:HOH:O	1.55	1.04
1:B:740:GLU:HG2	1:B:833:MET:SD	1.99	1.02
1:A:423:ALA:O	1:A:424:SER:HB3	1.69	0.92
1:A:618:THR:OG1	1:A:688:THR:HG22	1.71	0.89
1:B:982:ARG:CZ	8:B:4101:HOH:O	2.06	0.87
1:A:565:LYS:H	1:A:565:LYS:HD3	1.45	0.81
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.45	0.81
1:A:231:GLU:OE2	1:A:680:ARG:NH2	2.13	0.81
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.46	0.78
1:A:565:LYS:N	1:A:565:LYS:HD3	1.98	0.78
1:B:982:ARG:NH2	8:B:4101:HOH:O	2.13	0.78
1:A:426:ARG:HH11	1:A:426:ARG:HB3	1.51	0.75
1:B:241:MET:HE2	1:B:283:ILE:HG21	1.68	0.75
1:A:709:GLY:O	1:A:899:ARG:NH2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLN:HE21	1:B:132:GLU:H	1.34	0.74
1:B:472:GLN:HA	1:B:475:LYS:HD3	1.70	0.73
1:A:130:GLN:HE21	1:A:132:GLU:H	1.33	0.73
1:A:446:ILE:HD12	1:A:534:MET:HB2	1.70	0.72
1:A:423:ALA:O	1:A:424:SER:CB	2.37	0.72
1:A:446:ILE:HD12	1:A:534:MET:CB	2.21	0.70
1:B:271:ASN:HB2	1:B:683:ARG:NH1	2.05	0.70
1:A:388:PHE:HA	1:A:396:LEU:HG	1.75	0.69
1:B:981:LYS:O	1:B:985:GLU:HG2	1.93	0.69
1:A:812:LEU:HD11	1:A:825:CYS:CB	2.24	0.68
1:B:699:GLN:O	1:B:703:ASN:HB2	1.94	0.68
1:A:618:THR:OG1	1:A:688:THR:CG2	2.42	0.67
1:B:1283:ALA:HA	1:B:1288:ASN:HD21	1.59	0.67
1:A:371:LEU:CD2	1:A:406:ILE:HG23	2.26	0.66
1:A:421:LYS:HD2	8:A:3146:HOH:O	1.97	0.64
1:B:191:SER:OG	1:B:192:PRO:HD3	1.98	0.64
1:A:565:LYS:N	1:A:565:LYS:CD	2.61	0.63
1:A:812:LEU:HD11	1:A:825:CYS:HB3	1.81	0.62
1:A:240:THR:HG22	1:A:243:GLU:H	1.64	0.62
1:B:552:ASP:HB3	1:B:553:PRO:HD2	1.83	0.61
1:B:58:TYR:CE2	1:B:219:LYS:HD3	2.36	0.60
1:B:606:ARG:HD3	1:B:679:GLN:HA	1.82	0.60
1:A:371:LEU:HD23	1:A:406:ILE:HG23	1.84	0.59
1:B:1250:LYS:HG3	1:B:1251:ARG:H	1.67	0.59
1:A:138:ILE:HD12	1:A:163:ALA:HB2	1.83	0.58
1:A:812:LEU:HD11	1:A:825:CYS:HB2	1.87	0.57
1:B:336:PHE:HD1	1:B:336:PHE:O	1.88	0.56
1:A:1286:GLY:O	1:A:1287:ASP:HB3	2.05	0.56
1:A:63:ASN:O	1:A:64:LYS:HB3	2.05	0.56
1:B:157:GLN:HE22	1:B:558:GLN:HE22	1.53	0.56
1:A:539:ASP:OD1	1:A:540:PRO:HD2	2.05	0.56
1:B:1032:THR:HG21	8:B:4364:HOH:O	2.06	0.55
1:B:1032:THR:CG2	1:B:1065:GLU:O	2.55	0.55
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	2.04	0.55
1:B:1288:ASN:O	1:B:1289:ALA:CB	2.55	0.55
1:A:532:GLU:OE1	1:A:537:LYS:HG2	2.07	0.54
1:A:812:LEU:HD21	1:A:825:CYS:N	2.22	0.54
1:B:271:ASN:HB2	1:B:683:ARG:CZ	2.37	0.54
1:A:446:ILE:O	1:A:446:ILE:CG2	2.55	0.54
1:B:1288:ASN:O	1:B:1289:ALA:HB3	2.07	0.54
1:B:271:ASN:ND2	1:B:271:ASN:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:THR:HG22	1:A:907:SER:OG	2.08	0.53
1:A:1032:THR:CG2	1:A:1065:GLU:O	2.58	0.52
1:A:280:PRO:HB2	1:A:286:LEU:HD23	1.91	0.51
1:A:852:LYS:CE	1:A:852:LYS:HA	2.41	0.51
1:A:1032:THR:HG23	1:A:1065:GLU:O	2.11	0.51
1:A:392:TYR:OH	1:A:429:ASP:OD2	2.25	0.50
1:B:472:GLN:HE22	1:B:475:LYS:NZ	2.09	0.50
1:A:240:THR:CG2	1:A:242:GLU:HB2	2.41	0.50
1:B:552:ASP:HB3	1:B:553:PRO:CD	2.41	0.50
1:B:969:ASP:HA	1:B:972:ILE:CG1	2.42	0.49
1:A:426:ARG:HH11	1:A:426:ARG:CB	2.24	0.49
1:A:555:ALA:O	1:A:1238:GLU:HA	2.13	0.48
1:A:255:LYS:HE2	1:A:274:PHE:CE1	2.48	0.48
1:A:721:LYS:O	1:A:725:GLU:HG3	2.13	0.48
1:A:866:ASN:C	1:A:866:ASN:HD22	2.16	0.48
1:A:1080:SER:O	1:A:1258:ALA:HB1	2.14	0.47
1:B:1032:THR:HG23	1:B:1065:GLU:O	2.14	0.47
1:A:764:VAL:O	1:A:791:VAL:HG22	2.14	0.47
1:A:64:LYS:HE3	1:A:66:VAL:HG12	1.96	0.47
1:A:792:LYS:HE3	1:B:756:GLU:OE1	2.15	0.47
1:A:565:LYS:H	1:A:565:LYS:CD	2.13	0.47
1:B:975:SER:O	1:B:980:ARG:HD3	2.14	0.47
1:B:306:LEU:O	1:B:310:VAL:HG13	2.15	0.46
1:A:361:ASN:N	1:A:362:PRO:CD	2.79	0.46
1:A:190:LEU:HD13	1:A:191:SER:H	1.80	0.46
1:A:571:ASP:OD1	1:A:1052:ARG:HD3	2.15	0.46
1:B:900:ILE:HD12	1:B:900:ILE:N	2.31	0.46
1:A:446:ILE:HD12	1:A:534:MET:HB3	1.94	0.46
1:B:557:VAL:HG13	1:B:1240:ARG:HG2	1.97	0.46
1:B:337:ALA:HB2	5:B:4004:FAD:C6	2.46	0.46
1:B:335:TRP:CE3	1:B:335:TRP:HA	2.50	0.46
1:B:911:PHE:O	1:B:912:ARG:C	2.53	0.46
1:A:863:HIS:O	1:A:898:GLY:HA2	2.16	0.45
1:B:1151:HIS:NE2	1:B:1251:ARG:HG3	2.31	0.45
1:A:749:THR:O	1:A:812:LEU:HD22	2.15	0.45
1:A:740:GLU:HG3	1:A:833:MET:CE	2.47	0.45
1:B:336:PHE:CD1	1:B:336:PHE:O	2.67	0.45
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.17	0.45
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	1.99	0.45
1:A:387:THR:O	1:A:396:LEU:HD21	2.16	0.45
1:A:740:GLU:HG2	1:A:1211:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.17	0.44
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.17	0.44
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.33	0.43
1:A:164:LYS:C	1:A:165:ASP:OD1	2.56	0.43
1:A:345:ALA:HB1	5:A:3005:FAD:H4'	2.00	0.43
1:A:302:CYS:HB2	1:A:347:ILE:HD11	2.01	0.43
1:B:812:LEU:HD21	1:B:823:VAL:O	2.19	0.43
1:A:900:ILE:HD12	1:A:900:ILE:C	2.39	0.43
1:A:99:PRO:O	1:A:103:ARG:HG3	2.19	0.43
1:A:679:GLN:HE21	1:A:683:ARG:NH2	2.17	0.43
1:A:356:PRO:HD2	1:A:429:ASP:OD1	2.19	0.42
1:A:617:ILE:HG23	1:A:687:ILE:CD1	2.49	0.42
1:B:812:LEU:HD11	1:B:825:CYS:CB	2.50	0.42
1:A:749:THR:O	1:A:812:LEU:CD2	2.68	0.42
1:A:571:ASP:CG	1:A:1052:ARG:HD3	2.41	0.42
1:B:473:LEU:O	1:B:474:SER:HB2	2.20	0.42
1:A:995:LYS:HZ3	1:A:1284:GLN:HE21	1.68	0.41
1:B:393:ARG:NH2	1:B:429:ASP:OD1	2.45	0.41
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.18	0.41
1:B:968:TRP:O	1:B:972:ILE:HG12	2.21	0.41
1:B:1151:HIS:O	1:B:1251:ARG:HD3	2.21	0.41
1:B:934:CYS:HB3	1:B:936:LEU:HD12	2.02	0.41
1:A:1102:GLU:HB3	1:A:1103:PRO:HD3	2.02	0.41
1:B:1204:GLY:HA3	1:B:1209:GLU:OE2	2.21	0.41
1:B:969:ASP:HA	1:B:972:ILE:HG12	2.02	0.41
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.03	0.41
1:A:446:ILE:HG22	1:A:446:ILE:O	2.19	0.41
1:B:806:THR:O	1:B:810:THR:HG23	2.21	0.41
1:A:599:TYR:HA	1:B:599:TYR:HA	2.03	0.41
1:A:975:SER:O	1:A:980:ARG:HD3	2.21	0.41
1:B:866:ASN:HD22	1:B:866:ASN:C	2.24	0.40
1:A:153:ARG:HD2	1:A:153:ARG:C	2.42	0.40
1:B:99:PRO:O	1:B:103:ARG:HG3	2.22	0.40
1:B:134:THR:OG1	1:B:137:GLU:HG3	2.22	0.40
1:A:241:MET:CE	1:A:245:LEU:HD11	2.51	0.40
1:A:447:GLU:HA	1:A:475:LYS:O	2.21	0.40
1:B:345:ALA:HB1	5:B:4004:FAD:H4'	2.04	0.40
1:B:733:GLU:HA	1:B:844:ALA:O	2.22	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	1285/1315 (98%)	1239 (96%)	38 (3%)	8 (1%)	28	21
1	B	1282/1315 (98%)	1242 (97%)	32 (2%)	8 (1%)	28	21
All	All	2567/2630 (98%)	2481 (97%)	70 (3%)	16 (1%)	28	21

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	B	1251	ARG
1	B	1287	ASP
1	B	1289	ALA
1	A	424	SER
1	B	912	ARG
1	A	797	GLY
1	A	912	ARG
1	A	1287	ASP
1	B	797	GLY
1	B	887	ASN
1	A	474	SER
1	A	552	ASP
1	A	887	ASN
1	B	556	ASN

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	1088/1109 (98%)	1029 (95%)	59 (5%)	26	20
1	B	1085/1109 (98%)	1042 (96%)	43 (4%)	36	32
All	All	2173/2218 (98%)	2071 (95%)	102 (5%)	30	26

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	61	LEU
1	A	64	LYS
1	A	70	VAL
1	A	83	VAL
1	A	94	THR
1	A	96	LYS
1	A	164	LYS
1	A	190	LEU
1	A	221	THR
1	A	240	THR
1	A	242	GLU
1	A	247	LEU
1	A	270	LYS
1	A	271	ASN
1	A	286	LEU
1	A	290	VAL
1	A	297	SER
1	A	306	LEU
1	A	313	GLU
1	A	347	ILE
1	A	383	ARG
1	A	396	LEU
1	A	404	LEU
1	A	406	ILE
1	A	424	SER
1	A	425	ARG
1	A	426	ARG
1	A	447	GLU
1	A	483	GLN
1	A	494	GLN
1	A	512	LEU
1	A	565	LYS
1	A	626	LYS
1	A	640	VAL

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Mol	Chain	Res	Type
1	A	683	ARG
1	A	686	LYS
1	A	687	ILE
1	A	688	THR
1	A	743	TYR
1	A	752	VAL
1	A	807	VAL
1	A	818	LYS
1	A	852	LYS
1	A	866	ASN
1	A	870	THR
1	A	900	ILE
1	A	911	PHE
1	A	1011	LEU
1	A	1031	LEU
1	A	1032	THR
1	A	1052	ARG
1	A	1085	LEU
1	A	1106	LYS
1	A	1108	LYS
1	A	1134	LYS
1	A	1251	ARG
1	A	1288	ASN
1	A	1315	LEU
1	B	28	VAL
1	B	61	LEU
1	B	62	GLN
1	B	64	LYS
1	B	70	VAL
1	B	164	LYS
1	B	201	LYS
1	B	216	LEU
1	B	219	LYS
1	B	247	LEU
1	B	270	LYS
1	B	271	ASN
1	B	280	PRO
1	B	317	LYS
1	B	336	PHE
1	B	383	ARG
1	B	400	GLU
1	B	476	SER

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Mol	Chain	Res	Type
1	B	512	LEU
1	B	531	LEU
1	B	550	GLN
1	B	551	LYS
1	B	566	ASP
1	B	622	THR
1	B	683	ARG
1	B	720	LYS
1	B	743	TYR
1	B	752	VAL
1	B	812	LEU
1	B	866	ASN
1	B	911	PHE
1	B	981	LYS
1	B	985	GLU
1	B	1011	LEU
1	B	1031	LEU
1	B	1032	THR
1	B	1051	SER
1	B	1099	LYS
1	B	1102	GLU
1	B	1143	GLU
1	B	1145	ASN
1	B	1239	PHE
1	B	1291	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	271	ASN
1	A	321	GLN
1	A	350	ASN
1	A	472	GLN
1	A	583	ASN
1	A	585	GLN
1	A	728	ASN
1	A	866	ASN
1	A	1088	GLN
1	A	1145	ASN
1	A	1284	GLN
1	A	1285	HIS

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Mol	Chain	Res	Type
1	A	1288	ASN
1	B	62	GLN
1	B	130	GLN
1	B	157	GLN
1	B	223	GLN
1	B	271	ASN
1	B	291	HIS
1	B	350	ASN
1	B	472	GLN
1	B	583	ASN
1	B	642	ASN
1	B	703	ASN
1	B	866	ASN
1	B	1088	GLN
1	B	1145	ASN
1	B	1284	GLN
1	B	1288	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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
2	FES	A	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	A	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
3	BCT	A	3003	-	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	A	3005	-	51,58,58	1.59	12 (23%)	54,89,89	2.69	19 (35%)
6	URC	A	3006	-	12,13,13	4.23	6 (50%)	12,19,19	4.45	7 (58%)
7	GOL	A	3007	-	5,5,5	0.67	0	5,5,5	0.66	0
2	FES	B	4001	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	B	4002	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FAD	B	4004	-	51,58,58	1.92	18 (35%)	54,89,89	2.47	13 (24%)
3	BCT	B	4005	-	0,3,3	0.00	-	0,3,3	0.00	-
6	URC	B	4006	-	12,13,13	3.57	8 (66%)	12,19,19	5.24	8 (66%)
7	GOL	B	4007	-	5,5,5	0.60	0	5,5,5	0.35	0
7	GOL	B	4008	-	5,5,5	0.50	0	5,5,5	0.32	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	FES	A	3001	1	-	0/0/4/4	0/1/1/1
2	FES	A	3002	1	-	0/0/4/4	0/1/1/1
3	BCT	A	3003	-	-	0/0/0/0	0/0/0/0
5	FAD	A	3005	-	-	0/28/50/50	0/6/6/6
6	URC	A	3006	-	-	0/0/0/0	0/2/2/2
7	GOL	A	3007	-	-	0/4/4/4	0/0/0/0
2	FES	B	4001	1	-	0/0/4/4	0/1/1/1
2	FES	B	4002	1	-	0/0/4/4	0/1/1/1
5	FAD	B	4004	-	-	0/28/50/50	0/6/6/6
3	BCT	B	4005	-	-	0/0/0/0	0/0/0/0
6	URC	B	4006	-	-	0/0/0/0	0/2/2/2
7	GOL	B	4007	-	-	0/4/4/4	0/0/0/0
7	GOL	B	4008	-	-	0/4/4/4	0/0/0/0

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3006	URC	C4-N3	-9.60	1.35	1.46
6	A	3006	URC	C4-N9	-8.20	1.34	1.44
6	B	4006	URC	C4-N3	-7.61	1.37	1.46
5	B	4004	FAD	C1'-N10	-6.92	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	4006	URC	C4-N9	-6.75	1.36	1.44
6	A	3006	URC	C5-N7	-4.32	1.36	1.45
6	B	4006	URC	C5-N7	-3.18	1.38	1.45
5	B	4004	FAD	C6-C5X	-3.00	1.37	1.41
5	B	4004	FAD	PA-O2A	-3.00	1.40	1.55
5	B	4004	FAD	C2-N1	-2.79	1.32	1.38
5	B	4004	FAD	P-O1P	-2.77	1.40	1.50
5	B	4004	FAD	C2B-C1B	-2.67	1.49	1.53
6	A	3006	URC	C5-C6	-2.63	1.48	1.53
5	B	4004	FAD	C2-N3	-2.57	1.33	1.38
5	B	4004	FAD	C5A-N7A	-2.51	1.30	1.39
5	B	4004	FAD	PA-O1A	-2.42	1.41	1.50
5	A	3005	FAD	C2B-C3B	-2.40	1.47	1.53
5	B	4004	FAD	P-O2P	-2.29	1.43	1.55
5	A	3005	FAD	C2-N1	-2.28	1.33	1.38
5	A	3005	FAD	C2'-C3'	-2.25	1.49	1.53
5	A	3005	FAD	C2B-C1B	-2.21	1.50	1.53
5	B	4004	FAD	C2'-C3'	-2.14	1.49	1.53
5	B	4004	FAD	C5X-N5	-2.11	1.32	1.35
6	B	4006	URC	C5-C6	-2.11	1.49	1.53
5	B	4004	FAD	O4B-C4B	-2.09	1.40	1.45
5	A	3005	FAD	O2'-C2'	2.13	1.48	1.43
5	B	4004	FAD	C5A-C4A	2.16	1.45	1.40
6	B	4006	URC	O13-C6	2.21	1.27	1.23
5	A	3005	FAD	O4B-C1B	2.32	1.44	1.41
5	A	3005	FAD	C2A-N3A	2.38	1.36	1.32
5	A	3005	FAD	C5A-C4A	2.41	1.45	1.40
5	B	4004	FAD	C8-C7	2.46	1.47	1.41
5	B	4004	FAD	C4X-C10	2.48	1.45	1.41
5	A	3005	FAD	C8-C7	2.56	1.47	1.41
5	B	4004	FAD	C9A-C5X	2.58	1.47	1.42
6	B	4006	URC	C8-N9	2.68	1.39	1.35
6	B	4006	URC	O11-C2	2.69	1.29	1.23
5	B	4004	FAD	C4-C4X	3.07	1.47	1.41
5	A	3005	FAD	C9A-C5X	3.09	1.48	1.42
5	A	3005	FAD	C9A-N10	3.37	1.43	1.38
6	A	3006	URC	O13-C6	3.56	1.30	1.23
6	B	4006	URC	O24-C8	3.56	1.31	1.23
6	A	3006	URC	O24-C8	3.72	1.31	1.23
5	A	3005	FAD	C4X-C10	3.83	1.47	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	4006	URC	C4-N9-C8	-10.48	105.77	112.89
6	A	3006	URC	C4-N9-C8	-8.53	107.09	112.89
5	A	3005	FAD	C4-C4X-C10	-6.73	114.52	119.96
5	B	4004	FAD	C4-C4X-C10	-5.47	115.54	119.96
5	B	4004	FAD	C4X-C10-N10	-4.52	117.38	120.52
5	B	4004	FAD	N3A-C2A-N1A	-4.41	125.02	128.86
5	A	3005	FAD	N3A-C2A-N1A	-4.18	125.22	128.86
5	A	3005	FAD	C4X-C4-N3	-4.11	117.63	123.48
5	B	4004	FAD	C4X-C4-N3	-4.04	117.73	123.48
5	A	3005	FAD	O3'-C3'-C2'	-3.87	99.22	108.82
5	A	3005	FAD	C4X-C10-N10	-3.83	117.86	120.52
5	B	4004	FAD	O3'-C3'-C2'	-3.75	99.53	108.82
6	B	4006	URC	O24-C8-N9	-3.63	120.92	125.90
5	B	4004	FAD	C4A-C5A-N7A	-3.00	106.51	109.41
5	A	3005	FAD	C1B-N9A-C4A	-2.83	121.75	126.64
6	B	4006	URC	O24-C8-N7	-2.53	122.43	125.90
6	A	3006	URC	O11-C2-N3	-2.45	117.73	122.89
6	B	4006	URC	O11-C2-N3	-2.43	117.78	122.89
6	A	3006	URC	O24-C8-N9	-2.41	122.60	125.90
6	A	3006	URC	O24-C8-N7	-2.39	122.62	125.90
5	A	3005	FAD	C4A-C5A-N7A	-2.34	107.15	109.41
5	A	3005	FAD	C4B-O4B-C1B	-2.19	107.44	109.77
5	B	4004	FAD	C9A-C5X-N5	-2.17	119.01	122.24
6	B	4006	URC	C6-N1-C2	-2.06	123.34	126.23
5	A	3005	FAD	C6-C5X-C9A	2.03	121.64	119.00
5	A	3005	FAD	C2B-C3B-C4B	2.13	106.77	102.62
5	B	4004	FAD	O5B-C5B-C4B	2.15	116.62	109.00
5	B	4004	FAD	O2'-C2'-C1'	2.18	114.83	109.79
5	A	3005	FAD	O2'-C2'-C1'	2.20	114.89	109.79
5	A	3005	FAD	N6A-C6A-N1A	2.37	123.46	118.77
5	A	3005	FAD	C10-C4X-N5	2.45	123.41	120.59
5	A	3005	FAD	O4'-C4'-C3'	2.87	116.22	109.09
5	A	3005	FAD	C5X-C9A-N10	2.91	119.82	117.66
5	A	3005	FAD	C4-C4X-N5	3.09	122.07	118.68
5	A	3005	FAD	C4X-N5-C5X	3.18	120.12	116.76
5	B	4004	FAD	C1'-N10-C9A	3.97	121.99	118.35
5	B	4004	FAD	C4-C4X-N5	4.06	123.13	118.68
5	A	3005	FAD	C1'-N10-C9A	4.73	122.68	118.35
5	B	4004	FAD	C4X-N5-C5X	5.97	123.07	116.76
6	A	3006	URC	C5-C4-N9	6.30	105.56	102.64
6	B	4006	URC	C5-C4-N9	6.31	105.56	102.64
6	A	3006	URC	N1-C2-N3	6.71	123.13	116.14
6	B	4006	URC	N1-C2-N3	6.93	123.35	116.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	3006	URC	N7-C8-N9	7.44	114.58	108.85
6	B	4006	URC	N7-C8-N9	9.89	116.48	108.85
5	B	4004	FAD	C4-N3-C2	10.10	124.00	115.16
5	A	3005	FAD	C4-N3-C2	11.88	125.55	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3005	FAD	1	0
5	B	4004	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	1289/1315 (98%)	0.29	53 (4%) 38 38	17, 30, 51, 86	0
1	B	1286/1315 (97%)	0.06	33 (2%) 56 56	15, 24, 46, 85	0
All	All	2575/2630 (97%)	0.17	86 (3%) 47 47	15, 27, 49, 86	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	SER	6.4
1	A	1287	ASP	6.2
1	A	3	ALA	5.9
1	B	1289	ALA	5.7
1	A	1315	LEU	5.5
1	B	423	ALA	5.2
1	B	1286	GLY	5.2
1	A	165	ASP	5.0
1	B	1287	ASP	4.5
1	A	1111	GLY	4.4
1	A	550	GLN	4.1
1	A	290	VAL	4.0
1	B	1314	THR	3.9
1	B	1106	LYS	3.8
1	A	396	LEU	3.8
1	B	551	LYS	3.6
1	B	555	ALA	3.6
1	A	473	LEU	3.6
1	B	553	PRO	3.6
1	B	1288	ASN	3.3
1	B	1111	GLY	3.2
1	A	1288	ASN	3.2
1	B	530	ASP	3.1
1	B	549	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	377	GLY	3.1
1	A	190	LEU	3.1
1	B	428	ASP	3.0
1	B	552	ASP	3.0
1	B	218	LEU	2.9
1	A	1110	THR	2.9
1	B	550	GLN	2.9
1	A	687	ILE	2.8
1	A	474	SER	2.8
1	A	222	PRO	2.8
1	A	61	LEU	2.8
1	A	693	PRO	2.7
1	A	448	VAL	2.7
1	B	566	ASP	2.7
1	B	1108	LYS	2.7
1	B	565	LYS	2.6
1	A	800	GLY	2.6
1	A	566	ASP	2.6
1	B	532	GLU	2.6
1	A	551	LYS	2.6
1	A	191	SER	2.6
1	A	335	TRP	2.6
1	A	321	GLN	2.6
1	B	1110	THR	2.6
1	A	220	ASP	2.5
1	A	553	PRO	2.5
1	A	798	PHE	2.5
1	B	221	THR	2.4
1	A	470	PRO	2.4
1	B	220	ASP	2.4
1	B	529	ALA	2.4
1	A	742	PHE	2.4
1	A	686	LYS	2.4
1	B	1107	LYS	2.4
1	A	247	LEU	2.4
1	A	221	THR	2.4
1	B	1109	PRO	2.4
1	B	1105	LYS	2.3
1	A	466	LEU	2.3
1	A	1289	ALA	2.3
1	A	565	LYS	2.3
1	A	724	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	443	PRO	2.2
1	A	1314	THR	2.2
1	A	317	LYS	2.2
1	A	444	GLY	2.2
1	A	413	GLU	2.2
1	A	1264	LEU	2.1
1	A	224	LYS	2.1
1	A	723	PHE	2.1
1	B	548	LEU	2.1
1	B	1116	TRP	2.1
1	A	795	GLY	2.1
1	A	692	LEU	2.1
1	A	720	LYS	2.1
1	A	293	PRO	2.1
1	B	1102	GLU	2.0
1	A	1229	ILE	2.0
1	A	533	ASP	2.0
1	A	1036	THR	2.0
1	A	291	HIS	2.0
1	B	1143	GLU	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
7	GOL	A	3007	6/6	0.94	0.16	1.53	25,27,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	GOL	B	4008	6/6	0.94	0.11	0.72	23,27,28,28	0
3	BCT	B	4005	4/4	0.99	0.14	0.28	19,20,21,23	0
7	GOL	B	4007	6/6	0.95	0.10	-0.15	26,30,31,31	0
5	FAD	B	4004	53/53	0.97	0.10	-0.46	16,21,25,27	0
5	FAD	A	3005	53/53	0.97	0.10	-0.58	23,30,34,36	0
3	BCT	A	3003	4/4	0.99	0.12	-1.26	26,28,28,29	0
6	URC	B	4006	12/12	0.97	0.10	-1.40	22,24,28,29	0
6	URC	A	3006	12/12	0.96	0.11	-1.47	24,27,31,31	0
4	CA	A	3004	1/1	0.99	0.05	-1.90	34,34,34,34	0
2	FES	B	4001	4/4	0.99	0.04	-2.72	20,22,25,25	0
2	FES	A	3002	4/4	0.99	0.08	-2.85	19,21,24,25	0
2	FES	A	3001	4/4	0.99	0.05	-2.89	23,23,25,29	0
2	FES	B	4002	4/4	0.99	0.08	-2.93	15,15,18,18	0
4	CA	B	4003	1/1	1.00	0.04	-3.37	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.