Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:48 PM GMT

PDB ID	:	4PZF
Title	:	Berberine bridge enzyme G164A variant, a reticuline dehydrogenase
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Deposited on	:	2014-03-30
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

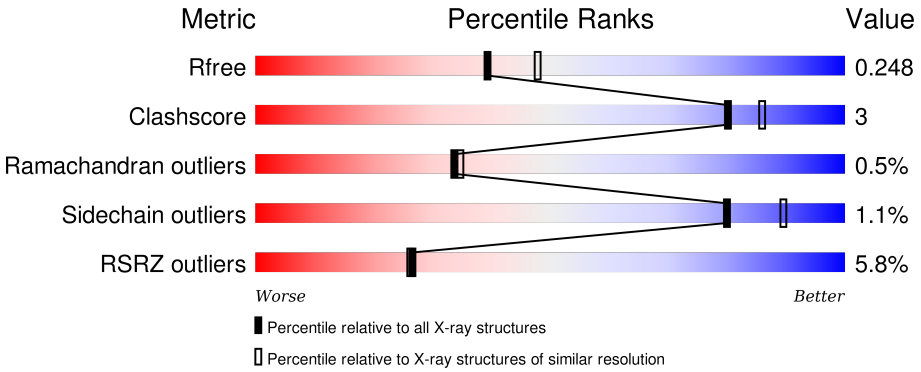
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 <=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	538	4% 86% 6% 7%
1	B	538	5% 85% 7% • 7%
1	C	538	7% 80% 12% • 8%
1	D	538	6% 84% 8% • 8%

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	NAG	A	602	-	-	-	X
5	SO4	B	605	-	-	X	-
5	SO4	D	606	-	-	-	X
5	SO4	D	607	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16476 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.

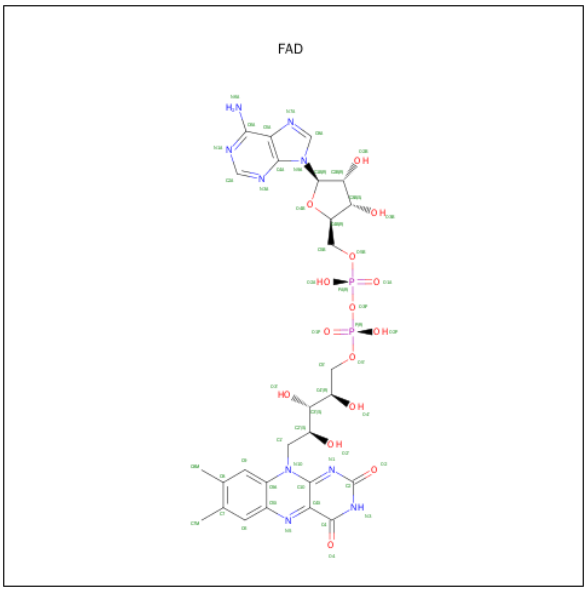
- Molecule 1 is a protein called Reticuline oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3935	2531	653	738	13			
1	B	498	Total	C	N	O	S	0	0	0
			3935	2531	654	737	13			
1	C	496	Total	C	N	O	S	0	0	0
			3916	2518	651	734	13			
1	D	497	Total	C	N	O	S	0	0	0
			3927	2527	652	735	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLU	LEU	SEE REMARK 999	UNP P30986
A	23	ALA	GLY	SEE REMARK 999	UNP P30986
A	164	ALA	GLY	ENGINEERED MUTATION	UNP P30986
B	22	GLU	LEU	SEE REMARK 999	UNP P30986
B	23	ALA	GLY	SEE REMARK 999	UNP P30986
B	164	ALA	GLY	ENGINEERED MUTATION	UNP P30986
C	22	GLU	LEU	SEE REMARK 999	UNP P30986
C	23	ALA	GLY	SEE REMARK 999	UNP P30986
C	164	ALA	GLY	ENGINEERED MUTATION	UNP P30986
D	22	GLU	LEU	SEE REMARK 999	UNP P30986
D	23	ALA	GLY	SEE REMARK 999	UNP P30986
D	164	ALA	GLY	ENGINEERED MUTATION	UNP P30986

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

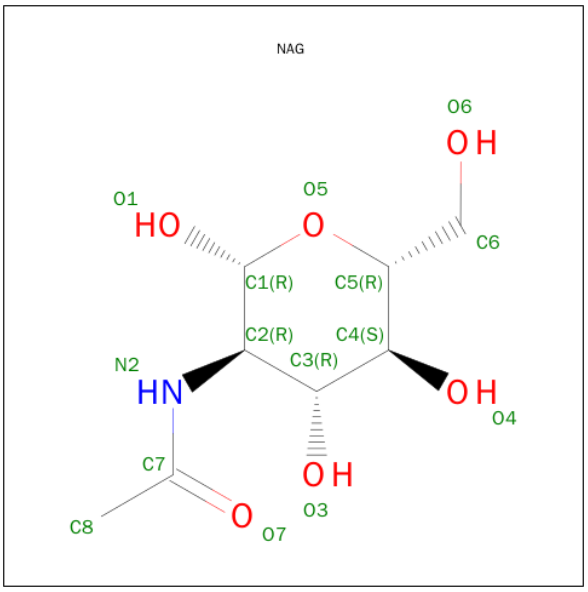


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

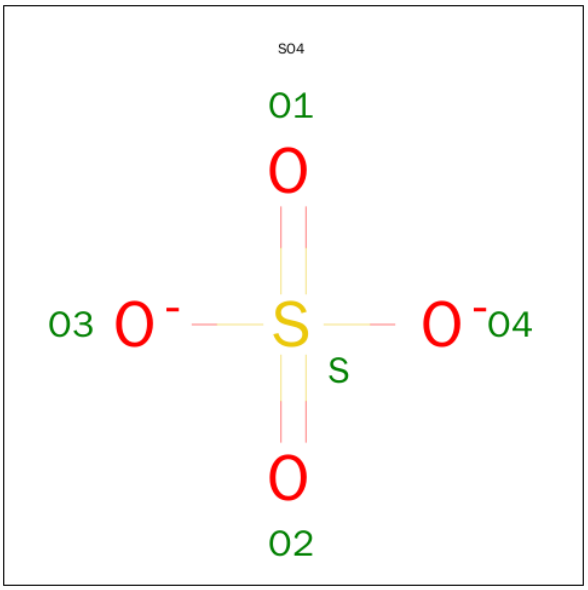
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



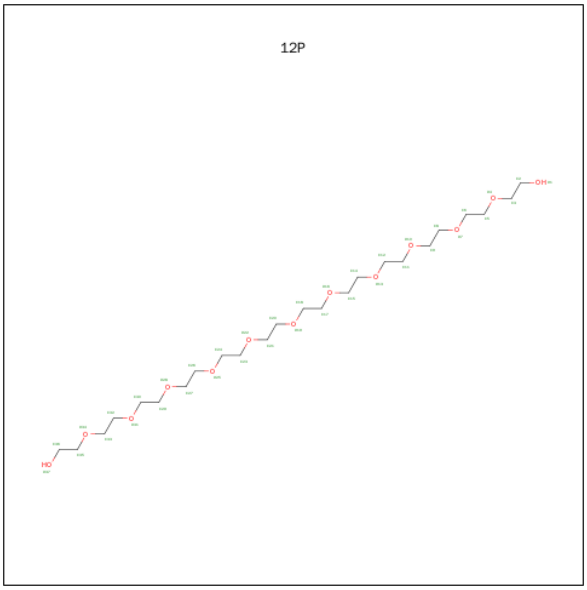
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

- Molecule 6 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula: $C_{24}H_{50}O_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 28 18 10	0	0
6	D	1	Total C O 22 14 8	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	105	Total O 105 105	0	0
7	B	71	Total O 71 71	0	0
7	C	72	Total O 72 72	0	0

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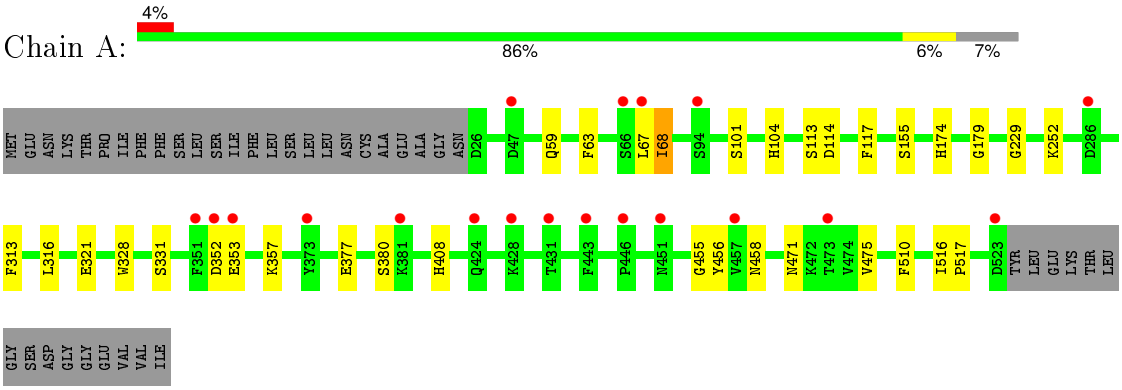
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	60	Total O 60 60	0	0

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 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.

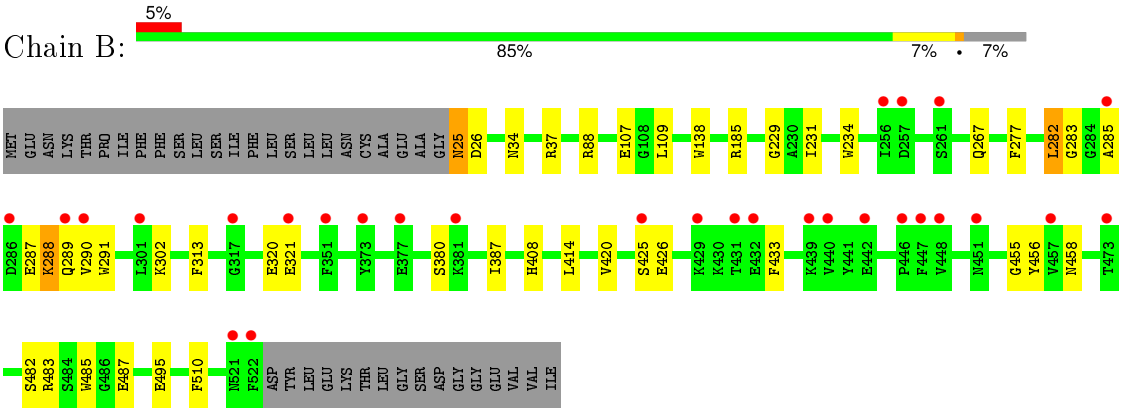
- Molecule 1: Reticuline oxidase

Chain A:



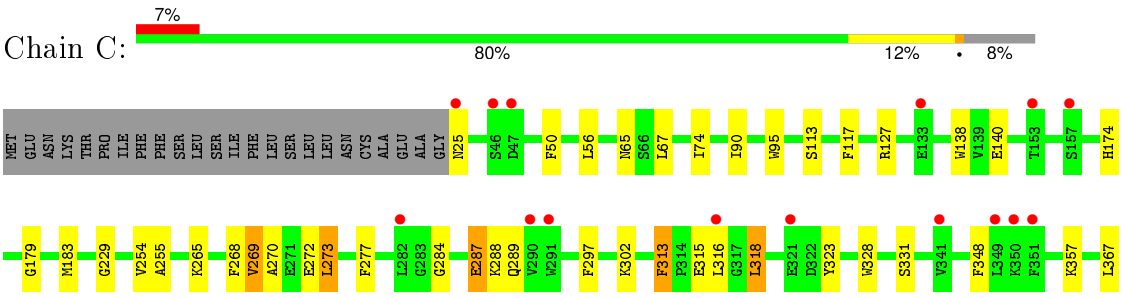
- Molecule 1: Reticuline oxidase

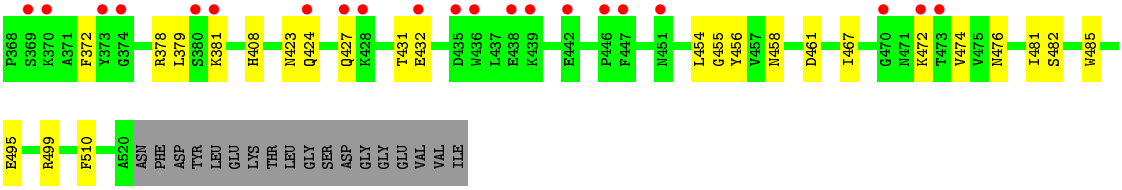
Chain B:



- Molecule 1: Reticuline oxidase

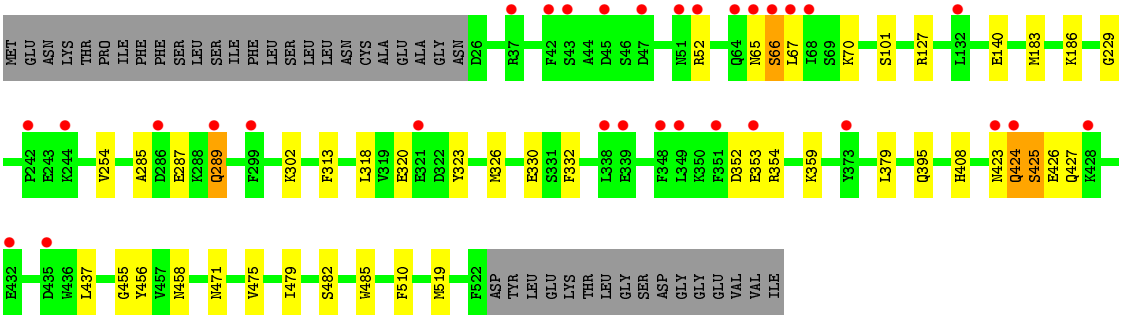
Chain C:





- Molecule 1: Reticuline oxidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	80.82Å 175.44Å 195.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.38 – 2.20 48.78 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.38-2.20) 61.9 (48.78-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 1.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.220 , 0.242 0.229 , 0.248	Depositor DCC
R_{free} test set	7017 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	10 of 272037 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16476	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.00 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0087e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 12P, NAG, FAD, SO4

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	0.25	0/4033	0.43	0/5465
1	B	0.25	0/4033	0.43	0/5465
1	C	0.25	0/4013	0.44	0/5438
1	D	0.25	0/4025	0.43	0/5454
All	All	0.25	0/16104	0.43	0/21822

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3935	0	3861	16	0
1	B	3935	0	3863	28	0
1	C	3916	0	3848	38	1
1	D	3927	0	3857	24	0
2	A	53	0	29	1	0
2	B	53	0	29	0	0
2	C	53	0	29	1	0
2	D	53	0	28	2	0
3	A	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	25	0	0
3	C	28	0	25	0	0
3	D	28	0	25	1	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	B	5	0	0	3	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
6	C	28	0	37	1	0
6	D	22	0	29	1	0
7	A	105	0	0	1	0
7	B	71	0	0	0	0
7	C	72	0	0	0	0
7	D	60	0	0	0	0
All	All	16476	0	15762	108	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (108) 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:483:ARG:NH2	1:B:495:GLU:OE2	2.11	0.83
1:D:52:ARG:NH2	3:D:603:NAG:O7	2.19	0.76
1:D:65:ASN:O	1:D:67:LEU:N	2.25	0.69
1:D:424:GLN:O	1:D:426:GLU:N	2.24	0.68
1:C:287:GLU:O	1:C:289:GLN:N	2.25	0.68
1:C:316:LEU:HB3	1:C:318:LEU:HD12	1.77	0.66
1:B:302:LYS:HE2	1:B:320:GLU:HG3	1.81	0.62
1:C:472:LYS:HE2	1:C:476:ASN:HD21	1.65	0.62
1:B:37:ARG:NH1	5:B:605:SO4:O4	2.32	0.62
1:C:472:LYS:O	1:C:476:ASN:ND2	2.32	0.62
1:D:66:SER:HA	1:D:70:LYS:HE2	1.83	0.61
1:C:269:VAL:HG12	1:C:273:LEU:HD11	1.84	0.59
1:D:352:ASP:OD1	1:D:353:GLU:N	2.36	0.58
1:B:288:LYS:H	1:B:380:SER:HB3	1.70	0.57
1:B:25:ASN:N	1:B:25:ASN:OD1	2.36	0.57
1:C:378:ARG:HA	1:C:381:LYS:HE2	1.86	0.56
1:D:359:LYS:HG3	1:D:437:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ARG:HG3	1:B:487:GLU:HG3	1.88	0.55
1:D:302:LYS:HD3	1:D:323:TYR:HB2	1.89	0.55
1:C:265:LYS:NZ	1:C:315:GLU:OE1	2.38	0.55
1:C:357:LYS:NZ	1:C:461:ASP:OD1	2.36	0.54
1:C:287:GLU:C	1:C:289:GLN:H	2.10	0.54
1:A:321:GLU:N	1:A:321:GLU:OE1	2.41	0.54
1:C:273:LEU:HD22	1:C:277:PHE:HB3	1.89	0.53
1:D:254:VAL:O	1:D:289:GLN:HG3	2.07	0.53
1:B:34:ASN:OD1	1:B:88:ARG:NH2	2.42	0.53
1:D:186:LYS:O	1:D:395:GLN:HG3	2.10	0.51
1:C:367:LEU:HB2	1:C:372:PHE:CE2	2.46	0.51
1:D:482:SER:HA	1:D:485:TRP:CZ2	2.45	0.51
1:A:377:GLU:O	1:A:380:SER:OG	2.27	0.51
1:B:285:ALA:HB2	1:B:290:VAL:HG13	1.93	0.51
1:C:456:TYR:CZ	1:C:458:ASN:HB2	2.46	0.50
1:D:479:ILE:HD11	1:D:519:MET:HA	1.92	0.50
1:D:456:TYR:CZ	1:D:458:ASN:HB2	2.46	0.50
1:B:456:TYR:CZ	1:B:458:ASN:HB2	2.46	0.49
1:A:229:GLY:HA2	1:A:510:PHE:CE2	2.47	0.49
1:C:423:ASN:OD1	1:C:424:GLN:N	2.39	0.49
1:D:302:LYS:HD2	1:D:320:GLU:HG3	1.95	0.49
1:C:472:LYS:HG2	1:C:476:ASN:HD21	1.78	0.49
1:D:127:ARG:NH1	1:D:140:GLU:OE1	2.46	0.49
1:D:229:GLY:HA2	1:D:510:PHE:CE2	2.48	0.49
1:B:229:GLY:HA2	1:B:510:PHE:CE2	2.48	0.48
1:D:352:ASP:OD2	1:D:354:ARG:NH2	2.43	0.48
1:B:408:HIS:HE1	1:B:455:GLY:O	1.97	0.48
1:B:138:TRP:HB3	6:D:605:12P:H172	1.96	0.48
1:B:267:GLN:HB2	1:B:414:LEU:HD11	1.96	0.47
1:A:63:PHE:HA	1:A:68:ILE:HD13	1.97	0.47
1:C:268:PHE:O	1:C:270:ALA:N	2.48	0.47
1:C:127:ARG:NH1	1:C:140:GLU:OE1	2.46	0.47
1:B:282:LEU:HB3	1:B:283:GLY:H	1.60	0.47
1:C:467:ILE:HG12	1:C:485:TRP:HZ2	1.79	0.47
1:A:328:TRP:O	1:A:331:SER:OG	2.28	0.47
1:B:282:LEU:O	1:B:387:ILE:HG13	2.14	0.47
1:C:302:LYS:HD2	1:C:323:TYR:O	2.15	0.46
1:C:90:ILE:HG23	1:C:95:TRP:HB2	1.96	0.46
1:C:254:VAL:HG12	1:C:255:ALA:O	2.14	0.46
1:D:354:ARG:HG2	1:D:423:ASN:N	2.30	0.46
1:D:408:HIS:HE1	1:D:455:GLY:O	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLY:HA2	1:B:291:TRP:O	2.16	0.45
1:C:269:VAL:O	1:C:272:GLU:N	2.45	0.45
1:C:65:ASN:OD1	1:C:67:LEU:HB2	2.16	0.45
1:D:318:LEU:HB3	1:D:323:TYR:HE2	1.82	0.45
1:C:482:SER:HA	1:C:485:TRP:CZ2	2.52	0.45
1:C:284:GLY:HA2	1:C:379:LEU:HD22	1.98	0.45
1:B:321:GLU:OE1	1:B:321:GLU:N	2.38	0.45
1:A:357:LYS:HD2	7:A:766:HOH:O	2.17	0.45
1:A:456:TYR:CZ	1:A:458:ASN:HB2	2.52	0.45
1:C:408:HIS:HE1	1:C:455:GLY:O	2.00	0.45
1:C:229:GLY:HA2	1:C:510:PHE:CE2	2.51	0.45
1:C:138:TRP:CG	6:C:605:12P:H171	2.52	0.45
1:A:352:ASP:OD1	1:A:353:GLU:N	2.50	0.45
1:A:252:LYS:NZ	1:A:316:LEU:O	2.50	0.45
1:D:183:MET:HG3	1:D:332:PHE:HZ	1.81	0.44
1:C:424:GLN:O	1:C:427:GLN:HB2	2.18	0.44
1:C:328:TRP:O	1:C:331:SER:OG	2.31	0.44
1:B:420:VAL:HG21	1:B:433:PHE:HB3	2.00	0.44
1:B:288:LYS:H	1:B:380:SER:CB	2.30	0.44
1:B:482:SER:HA	1:B:485:TRP:CZ2	2.53	0.44
1:B:287:GLU:C	1:B:289:GLN:H	2.21	0.44
1:C:270:ALA:HA	1:C:273:LEU:HD12	2.00	0.44
1:A:101:SER:HB3	2:A:601:FAD:O1P	2.18	0.43
1:C:474:VAL:HG13	1:C:481:ILE:HD12	1.99	0.43
1:D:471:ASN:O	1:D:475:VAL:HG23	2.18	0.43
1:B:185:ARG:NH1	1:B:277:PHE:O	2.51	0.43
1:D:101:SER:HB3	2:D:601:FAD:O1P	2.18	0.43
1:A:408:HIS:HE1	1:A:455:GLY:O	2.02	0.43
1:B:37:ARG:NH1	5:B:605:SO4:S	2.72	0.42
1:C:183:MET:HE2	1:C:297:PHE:CZ	2.54	0.42
1:A:174:HIS:CE1	1:A:179:GLY:HA2	2.54	0.42
1:D:285:ALA:HB2	1:D:379:LEU:O	2.19	0.42
1:C:113:SER:HB3	1:C:117:PHE:CD2	2.55	0.42
1:A:471:ASN:O	1:A:475:VAL:HG23	2.19	0.42
1:C:174:HIS:CE1	1:C:179:GLY:HA2	2.54	0.42
1:B:37:ARG:NH2	5:B:605:SO4:O1	2.47	0.42
1:C:50:PHE:CE1	1:C:74:ILE:HG13	2.54	0.42
1:C:313:PHE:CD1	1:C:316:LEU:HG	2.54	0.42
1:B:25:ASN:HB2	1:B:26:ASP:H	1.57	0.42
1:A:113:SER:HB3	1:A:117:PHE:CD2	2.55	0.41
1:C:408:HIS:CD2	1:C:454:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLN:HG3	1:A:104:HIS:CD2	2.56	0.41
1:C:56:LEU:HG	1:C:348:PHE:CE1	2.56	0.41
1:B:231:ILE:HG21	1:B:234:TRP:CE2	2.56	0.41
1:A:516:ILE:HA	1:A:517:PRO:HD3	1.87	0.41
1:B:107:GLU:HB2	1:B:109:LEU:HG	2.03	0.41
1:B:287:GLU:O	1:B:289:GLN:N	2.53	0.40
2:D:601:FAD:H1'2	2:D:601:FAD:H9	1.86	0.40
1:D:326:MET:HB2	1:D:330:GLU:HB2	2.02	0.40
2:C:601:FAD:H1'2	2:C:601:FAD:H9	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:GLU:OE1	1:C:499:ARG:NH1[3_556]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	496/538 (92%)	475 (96%)	19 (4%)	2 (0%)	39	42
1	B	496/538 (92%)	468 (94%)	27 (5%)	1 (0%)	52	59
1	C	494/538 (92%)	469 (95%)	22 (4%)	3 (1%)	30	29
1	D	495/538 (92%)	467 (94%)	24 (5%)	4 (1%)	24	22
All	All	1981/2152 (92%)	1879 (95%)	92 (5%)	10 (0%)	34	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ILE

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Mol	Chain	Res	Type
1	B	288	LYS
1	C	288	LYS
1	D	66	SER
1	D	424	GLN
1	A	67	LEU
1	C	269	VAL
1	C	287	GLU
1	D	425	SER
1	D	287	GLU

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	426/460 (93%)	423 (99%)	3 (1%)	88	94
1	B	426/460 (93%)	421 (99%)	5 (1%)	78	88
1	C	424/460 (92%)	418 (99%)	6 (1%)	74	85
1	D	425/460 (92%)	421 (99%)	4 (1%)	84	92
All	All	1701/1840 (92%)	1683 (99%)	18 (1%)	80	89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ASP
1	A	155	SER
1	A	313	PHE
1	B	25	ASN
1	B	282	LEU
1	B	313	PHE
1	B	425	SER
1	B	426	GLU
1	C	25	ASN
1	C	273	LEU
1	C	313	PHE
1	C	318	LEU

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Mol	Chain	Res	Type
1	C	431	THR
1	C	432	GLU
1	D	289	GLN
1	D	313	PHE
1	D	425	SER
1	D	427	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	408	HIS
1	B	25	ASN
1	B	55	HIS
1	B	408	HIS
1	B	459	HIS
1	C	55	HIS
1	C	408	HIS
1	C	459	HIS
1	C	476	ASN
1	D	408	HIS
1	D	459	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

8 carbohydrates 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	NAG	A	602	1,3	14,14,15	0.26	0	15,19,21	0.29	0
3	NAG	A	603	3	14,14,15	0.40	0	15,19,21	0.28	0
3	NAG	B	602	1,3	14,14,15	0.32	0	15,19,21	0.29	0
3	NAG	B	603	3	14,14,15	0.20	0	15,19,21	0.30	0
3	NAG	C	602	1,3	14,14,15	0.36	0	15,19,21	0.36	0
3	NAG	C	603	3	14,14,15	0.28	0	15,19,21	0.22	0
3	NAG	D	602	1,3	14,14,15	0.40	0	15,19,21	0.26	0
3	NAG	D	603	3	14,14,15	0.22	0	15,19,21	0.29	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
3	NAG	A	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	603	3	-	0/6/23/26	0/1/1/1
3	NAG	B	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	603	3	-	0/6/23/26	0/1/1/1
3	NAG	C	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	603	3	-	0/6/23/26	0/1/1/1
3	NAG	D	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	603	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	603	NAG	1	0

5.6 Ligand geometry (i)

15 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	$\#\|Z\| > 2$
2	FAD	A	601	1	48,58,58	1.37	6 (12%)	54,89,89	2.08	10 (18%)
4	NAG	A	604	1	14,14,15	0.20	0	15,19,21	0.40	0
2	FAD	B	601	1	48,58,58	1.35	5 (10%)	54,89,89	2.11	11 (20%)
4	NAG	B	604	1	14,14,15	0.29	0	15,19,21	0.24	0
5	SO4	B	605	-	4,4,4	0.21	0	6,6,6	0.09	0
2	FAD	C	601	1	48,58,58	1.34	5 (10%)	54,89,89	2.10	11 (20%)
4	NAG	C	604	1	14,14,15	0.40	0	15,19,21	0.27	0
6	12P	C	605	-	27,27,36	0.40	0	26,26,35	0.64	0
5	SO4	C	606	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	C	607	-	4,4,4	0.23	0	6,6,6	0.09	0
2	FAD	D	601	1	48,58,58	1.35	6 (12%)	54,89,89	2.13	10 (18%)
4	NAG	D	604	1	14,14,15	0.20	0	15,19,21	0.28	0
6	12P	D	605	-	21,21,36	0.42	0	20,20,35	0.49	0
5	SO4	D	606	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	D	607	-	4,4,4	0.21	0	6,6,6	0.09	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	FAD	A	601	1	-	0/30/50/50	0/6/6/6
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
2	FAD	B	601	1	-	0/30/50/50	0/6/6/6
4	NAG	B	604	1	-	0/6/23/26	0/1/1/1
5	SO4	B	605	-	-	0/0/0/0	0/0/0/0
2	FAD	C	601	1	-	0/30/50/50	0/6/6/6
4	NAG	C	604	1	-	0/6/23/26	0/1/1/1
6	12P	C	605	-	-	0/25/25/34	0/0/0/0
5	SO4	C	606	-	-	0/0/0/0	0/0/0/0
5	SO4	C	607	-	-	0/0/0/0	0/0/0/0
2	FAD	D	601	1	-	0/30/50/50	0/6/6/6
4	NAG	D	604	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	12P	D	605	-	-	0/19/19/34	0/0/0/0
5	SO4	D	606	-	-	0/0/0/0	0/0/0/0
5	SO4	D	607	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	O4B-C1B	2.02	1.43	1.41
2	A	601	FAD	O4B-C1B	2.21	1.44	1.41
2	B	601	FAD	C5A-C4A	2.99	1.47	1.40
2	D	601	FAD	C8-C7	3.02	1.49	1.41
2	C	601	FAD	C8-C7	3.04	1.49	1.41
2	B	601	FAD	C8-C7	3.05	1.49	1.41
2	D	601	FAD	C5A-C4A	3.08	1.47	1.40
2	A	601	FAD	C5A-C4A	3.09	1.47	1.40
2	A	601	FAD	C8-C7	3.12	1.49	1.41
2	C	601	FAD	C5A-C4A	3.14	1.47	1.40
2	C	601	FAD	C9A-C5X	3.40	1.49	1.42
2	B	601	FAD	C9A-C5X	3.44	1.49	1.42
2	A	601	FAD	C9A-C5X	3.46	1.49	1.42
2	D	601	FAD	C9A-C5X	3.47	1.49	1.42
2	A	601	FAD	C4-C4X	3.66	1.48	1.41
2	C	601	FAD	C4-C4X	3.68	1.48	1.41
2	B	601	FAD	C4-C4X	3.72	1.48	1.41
2	D	601	FAD	C4-C4X	3.73	1.48	1.41
2	A	601	FAD	C4X-C10	3.96	1.48	1.41
2	D	601	FAD	C4X-C10	3.98	1.48	1.41
2	C	601	FAD	C4X-C10	4.04	1.48	1.41
2	B	601	FAD	C4X-C10	4.08	1.48	1.41

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	FAD	N3A-C2A-N1A	-7.23	123.36	128.89
2	C	601	FAD	N3A-C2A-N1A	-6.92	123.60	128.89
2	D	601	FAD	N3A-C2A-N1A	-6.88	123.62	128.89
2	A	601	FAD	N3A-C2A-N1A	-6.66	123.80	128.89
2	D	601	FAD	C4-C4X-C10	-5.61	116.35	119.94
2	A	601	FAD	C4-C4X-C10	-5.26	116.57	119.94
2	C	601	FAD	C4-C4X-C10	-5.23	116.59	119.94
2	B	601	FAD	C4-C4X-C10	-4.96	116.77	119.94
2	B	601	FAD	C4X-C4-N3	-4.15	117.92	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	FAD	C4X-C4-N3	-4.11	117.97	123.59
2	C	601	FAD	C4X-C4-N3	-4.10	117.98	123.59
2	D	601	FAD	C4X-C4-N3	-4.01	118.10	123.59
2	C	601	FAD	C4A-C5A-N7A	-3.65	106.12	109.48
2	D	601	FAD	C4A-C5A-N7A	-3.51	106.25	109.48
2	A	601	FAD	C4A-C5A-N7A	-3.36	106.39	109.48
2	B	601	FAD	C4A-C5A-N7A	-3.20	106.54	109.48
2	C	601	FAD	P-O3P-PA	-2.92	124.54	132.73
2	B	601	FAD	P-O3P-PA	-2.86	124.70	132.73
2	A	601	FAD	P-O3P-PA	-2.70	125.14	132.73
2	D	601	FAD	C4X-C10-N10	-2.68	118.94	120.52
2	D	601	FAD	P-O3P-PA	-2.64	125.32	132.73
2	A	601	FAD	C4X-C10-N10	-2.58	119.00	120.52
2	B	601	FAD	C1B-N9A-C4A	-2.34	123.42	126.94
2	B	601	FAD	O3P-P-O5'	-2.32	96.78	102.94
2	A	601	FAD	O3P-P-O5'	-2.17	97.17	102.94
2	C	601	FAD	C4X-C10-N10	-2.09	119.29	120.52
2	B	601	FAD	C4X-C10-N10	-2.03	119.32	120.52
2	C	601	FAD	O3P-P-O5'	-2.03	97.55	102.94
2	D	601	FAD	C5X-C9A-N10	2.08	119.20	117.62
2	C	601	FAD	C5X-C9A-N10	2.37	119.42	117.62
2	C	601	FAD	C4-C4X-N5	2.66	121.95	118.72
2	B	601	FAD	C4-C4X-N5	2.77	122.08	118.72
2	A	601	FAD	C4-C4X-N5	2.90	122.24	118.72
2	D	601	FAD	C4-C4X-N5	2.99	122.35	118.72
2	C	601	FAD	C4X-N5-C5X	3.28	120.54	116.76
2	D	601	FAD	C4X-N5-C5X	3.47	120.75	116.76
2	B	601	FAD	C4X-N5-C5X	3.50	120.79	116.76
2	A	601	FAD	C4X-N5-C5X	3.52	120.81	116.76
2	C	601	FAD	C4-N3-C2	8.00	122.17	115.25
2	B	601	FAD	C4-N3-C2	8.01	122.17	115.25
2	A	601	FAD	C4-N3-C2	8.05	122.20	115.25
2	D	601	FAD	C4-N3-C2	8.15	122.29	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	605	SO4	3	0
2	C	601	FAD	1	0
6	C	605	12P	1	0
2	D	601	FAD	2	0
6	D	605	12P	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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	498/538 (92%)	-0.09	19 (3%)	44 43	28, 45, 76, 111	0
1	B	498/538 (92%)	0.22	29 (5%)	26 26	29, 56, 86, 114	0
1	C	496/538 (92%)	0.22	36 (7%)	18 17	30, 52, 80, 107	0
1	D	497/538 (92%)	0.11	31 (6%)	24 23	28, 50, 87, 114	0
All	All	1989/2152 (92%)	0.12	115 (5%)	26 26	28, 51, 84, 114	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	ASP	10.6
1	B	351	PHE	8.8
1	D	351	PHE	8.2
1	C	351	PHE	8.1
1	A	351	PHE	7.7
1	B	429	LYS	5.1
1	B	321	GLU	4.8
1	C	428	LYS	4.7
1	B	446	PRO	4.4
1	D	353	GLU	4.3
1	D	45	ASP	4.2
1	D	132	LEU	4.2
1	B	447	PHE	4.1
1	C	447	PHE	4.1
1	C	381	LYS	3.9
1	C	349	LEU	3.9
1	B	451	ASN	3.9
1	B	432	GLU	3.8
1	B	261	SER	3.7
1	D	64	GLN	3.7
1	B	286	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	448	VAL	3.5
1	B	522	PHE	3.5
1	A	67	LEU	3.5
1	B	257	ASP	3.5
1	A	424	GLN	3.5
1	C	373	TYR	3.5
1	C	427	GLN	3.4
1	C	432	GLU	3.4
1	D	68	ILE	3.4
1	D	428	LYS	3.3
1	D	321	GLU	3.2
1	A	473	THR	3.2
1	A	523	ASP	3.2
1	B	473	THR	3.2
1	D	339	GLU	3.2
1	D	299	PHE	3.1
1	C	473	THR	3.1
1	C	47	ASP	3.1
1	D	47	ASP	3.1
1	A	431	THR	3.1
1	D	65	ASN	3.1
1	C	291	TRP	3.1
1	B	439	LYS	3.0
1	D	424	GLN	3.0
1	B	431	THR	3.0
1	C	46	SER	2.9
1	C	157	SER	2.9
1	C	439	LYS	2.9
1	A	47	ASP	2.9
1	D	66	SER	2.9
1	C	370	LYS	2.8
1	B	373	TYR	2.8
1	A	451	ASN	2.8
1	B	256	ILE	2.8
1	B	521	ASN	2.8
1	B	381	LYS	2.7
1	D	423	ASN	2.7
1	C	435	ASP	2.7
1	C	369	SER	2.6
1	C	133	GLU	2.6
1	C	451	ASN	2.6
1	B	285	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	317	GLY	2.6
1	D	52	ARG	2.6
1	C	380	SER	2.5
1	C	350	LYS	2.5
1	D	435	ASP	2.5
1	C	341	VAL	2.5
1	A	66	SER	2.5
1	C	290	VAL	2.5
1	A	353	GLU	2.5
1	D	432	GLU	2.5
1	D	348	PHE	2.5
1	C	321	GLU	2.5
1	B	425	SER	2.5
1	C	446	PRO	2.4
1	D	51	ASN	2.4
1	D	67	LEU	2.4
1	D	373	TYR	2.4
1	B	289	GLN	2.3
1	D	286	ASP	2.3
1	D	37	ARG	2.3
1	C	438	GLU	2.3
1	D	244	LYS	2.3
1	D	42	PHE	2.3
1	C	472	LYS	2.3
1	C	442	GLU	2.2
1	A	428	LYS	2.2
1	A	446	PRO	2.2
1	C	374	GLY	2.2
1	A	94	SER	2.2
1	D	338	LEU	2.2
1	C	424	GLN	2.2
1	A	373	TYR	2.2
1	A	352	ASP	2.2
1	D	349	LEU	2.2
1	C	153	THR	2.2
1	B	457	VAL	2.1
1	A	443	PHE	2.1
1	C	470	GLY	2.1
1	B	440	VAL	2.1
1	C	316	LEU	2.1
1	C	282	LEU	2.1
1	C	25	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	242	PRO	2.1
1	D	43	SER	2.1
1	B	442	GLU	2.0
1	D	289	GLN	2.0
1	C	436	TRP	2.0
1	A	381	LYS	2.0
1	B	377	GLU	2.0
1	A	457	VAL	2.0
1	B	290	VAL	2.0
1	B	301	LEU	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)

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^{th} 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
3	NAG	A	602	14/15	0.85	0.18	2.06	50,55,60,65	0
3	NAG	B	602	14/15	0.81	0.17	1.73	56,63,69,70	0
3	NAG	C	602	14/15	0.84	0.17	1.43	54,63,67,68	0
3	NAG	D	602	14/15	0.67	0.26	1.40	63,73,79,80	0
3	NAG	B	603	14/15	0.80	0.18	-	68,73,81,84	0
3	NAG	C	603	14/15	0.85	0.23	-	63,70,78,80	0
3	NAG	D	603	14/15	0.81	0.30	-	72,86,97,100	0
3	NAG	A	603	14/15	0.81	0.25	-	50,69,79,80	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
5	SO4	D	607	5/5	0.84	0.19	4.99	46,50,55,64	5
5	SO4	D	606	5/5	0.81	0.19	3.61	48,52,57,59	5
5	SO4	C	606	5/5	0.97	0.17	1.33	60,62,73,73	0
5	SO4	C	607	5/5	0.92	0.17	0.54	56,57,63,69	5
2	FAD	C	601	53/53	0.95	0.18	0.07	28,38,50,53	0
2	FAD	A	601	53/53	0.96	0.16	0.04	24,31,41,44	0
2	FAD	B	601	53/53	0.96	0.18	-0.01	28,36,45,49	0
6	12P	D	605	22/37	0.82	0.10	-0.25	39,51,56,59	0
6	12P	C	605	28/37	0.85	0.11	-0.26	36,50,60,68	0
2	FAD	D	601	53/53	0.96	0.14	-0.33	26,34,47,50	0
5	SO4	B	605	5/5	0.97	0.09	-0.56	60,66,72,73	0
4	NAG	C	604	14/15	0.58	0.43	-	83,93,99,103	0
4	NAG	A	604	14/15	0.80	0.36	-	78,82,87,87	0
4	NAG	D	604	14/15	0.73	0.40	-	90,95,96,98	0
4	NAG	B	604	14/15	0.74	0.46	-	93,97,102,106	0

6.5 Other polymers (i)

There are no such residues in this entry.