



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2016 – 09:37 PM EST

PDB ID : 4GDC
Title : Crystal structure of oxidized *Aspergillus fumigatus* UDP-galactopyranose mutase complexed with NADPH
Authors : Tanner, J.J.; Dhatwalia, R.D.; Singh, H.
Deposited on : 2012-07-31
Resolution : 2.75 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

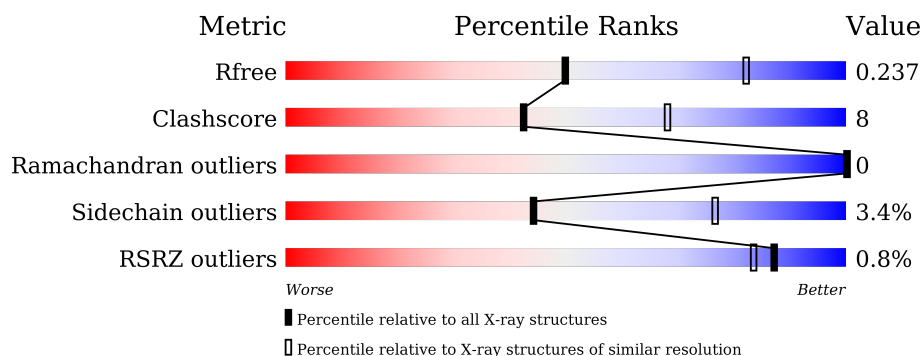
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	513	
1	B	513	
1	C	513	
1	D	513	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	C	604	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15449 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 UDP-galactopyranose mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3756	2396	632	707	21			
1	B	492	Total	C	N	O	S	0	0	0
			3748	2384	633	711	20			
1	C	501	Total	C	N	O	S	0	0	0
			3764	2394	635	716	19			
1	D	499	Total	C	N	O	S	0	0	0
			3740	2380	629	713	18			

There are 24 discrepancies between the modelled and reference sequences:

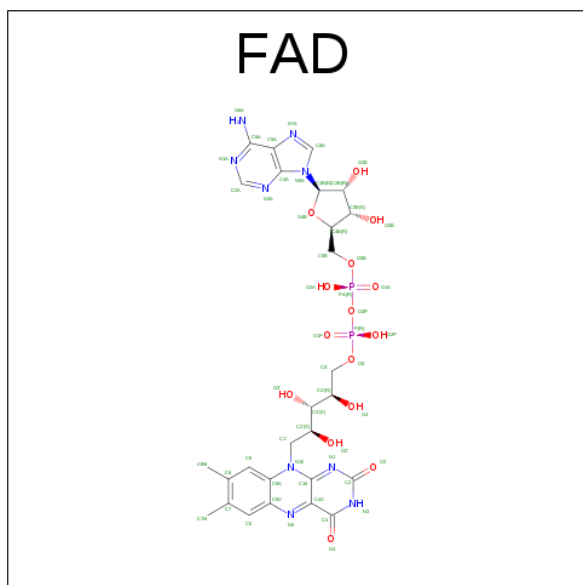
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	EXPRESSION TAG	UNP Q4W1X2
A	-1	ILE	-	EXPRESSION TAG	UNP Q4W1X2
A	0	ALA	-	EXPRESSION TAG	UNP Q4W1X2
A	344	ALA	LYS	ENGINEERED MUTATION	UNP Q4W1X2
A	345	ALA	LYS	ENGINEERED MUTATION	UNP Q4W1X2
A	429	THR	ALA	SEE REMARK 999	UNP Q4W1X2
B	-2	ALA	-	EXPRESSION TAG	UNP Q4W1X2
B	-1	ILE	-	EXPRESSION TAG	UNP Q4W1X2
B	0	ALA	-	EXPRESSION TAG	UNP Q4W1X2
B	344	ALA	LYS	ENGINEERED MUTATION	UNP Q4W1X2
B	345	ALA	LYS	ENGINEERED MUTATION	UNP Q4W1X2
B	429	THR	ALA	SEE REMARK 999	UNP Q4W1X2
C	-2	ALA	-	EXPRESSION TAG	UNP Q4W1X2
C	-1	ILE	-	EXPRESSION TAG	UNP Q4W1X2
C	0	ALA	-	EXPRESSION TAG	UNP Q4W1X2
C	344	ALA	LYS	ENGINEERED MUTATION	UNP Q4W1X2
C	345	ALA	LYS	ENGINEERED MUTATION	UNP Q4W1X2
C	429	THR	ALA	SEE REMARK 999	UNP Q4W1X2
D	-2	ALA	-	EXPRESSION TAG	UNP Q4W1X2
D	-1	ILE	-	EXPRESSION TAG	UNP Q4W1X2
D	0	ALA	-	EXPRESSION TAG	UNP Q4W1X2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	344	ALA	LYS	ENGINEERED MUTATION	UNP Q4W1X2
D	345	ALA	LYS	ENGINEERED MUTATION	UNP Q4W1X2
D	429	THR	ALA	SEE REMARK 999	UNP Q4W1X2

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



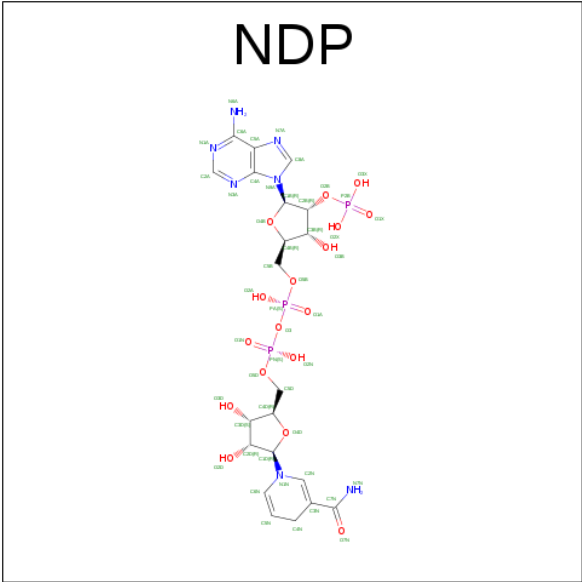
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

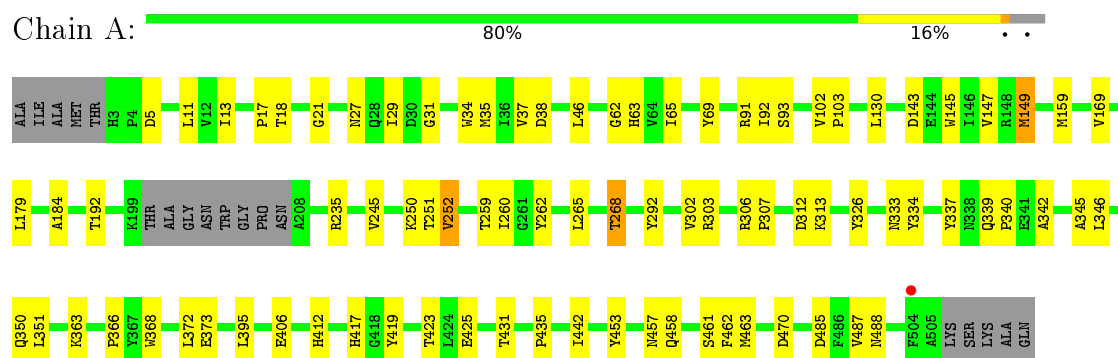
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	4	Total	O	0	0
			4	4		
5	C	3	Total	O	0	0
			3	3		
5	D	1	Total	O	0	0
			1	1		

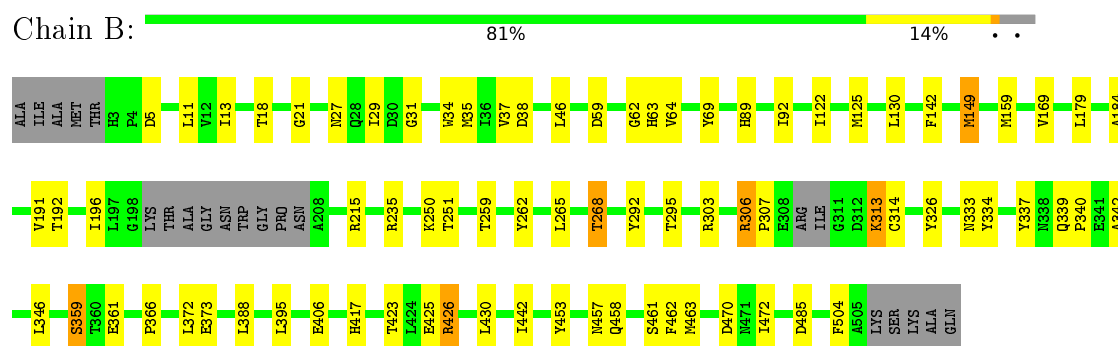
3 Residue-property plots

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.

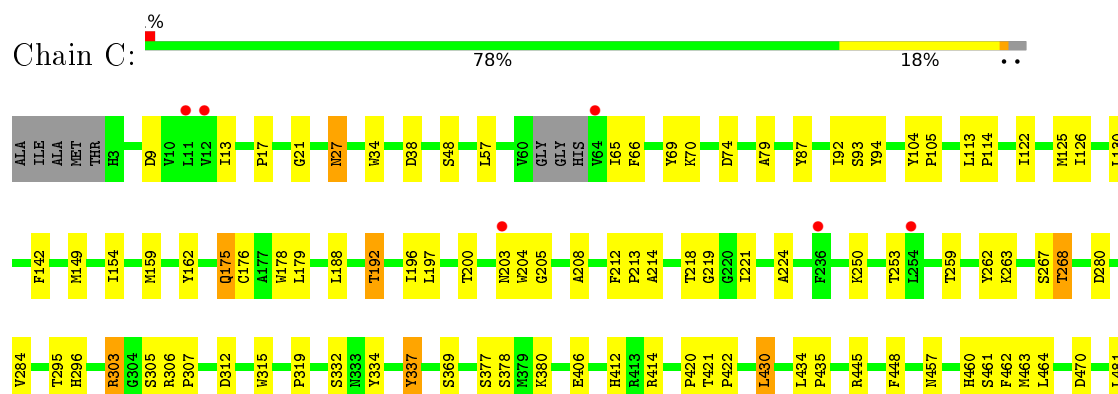
• Molecule 1: UDP-galactopyranose mutase

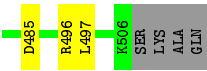


• Molecule 1: UDP-galactopyranose mutase

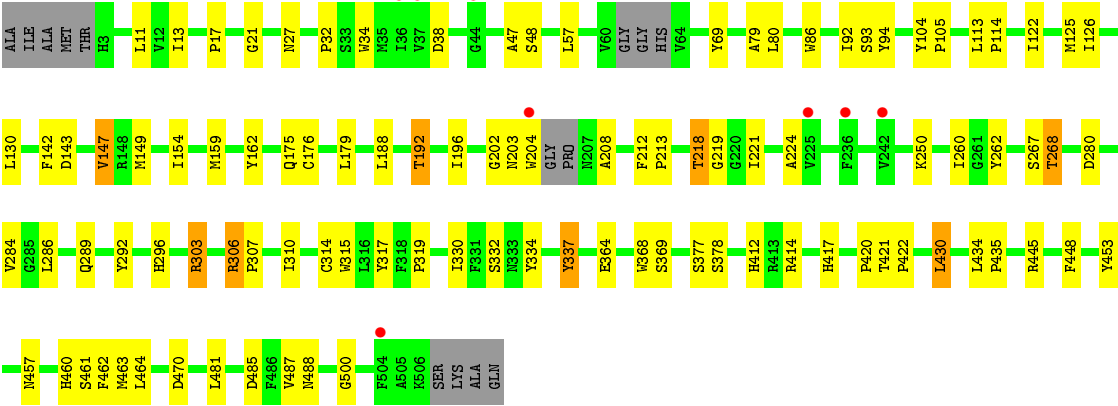
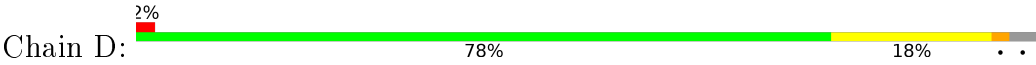


• Molecule 1: UDP-galactopyranose mutase





● Molecule 1: UDP-galactopyranose mutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	218.29 Å 218.29 Å 319.22 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	162.66 – 2.75 162.66 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (162.66-2.75) 99.7 (162.66-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.73 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.210 , 0.246 0.198 , 0.237	Depositor DCC
R_{free} test set	5834 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15449	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: NDP, SO4, 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	0.43	0/3850	0.60	0/5255
1	B	0.42	0/3840	0.59	0/5240
1	C	0.42	0/3859	0.63	3/5276 (0.1%)
1	D	0.41	0/3834	0.60	3/5243 (0.1%)
All	All	0.42	0/15383	0.60	6/21014 (0.0%)

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	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	ARG	NE-CZ-NH1	-13.44	113.58	120.30
1	C	303	ARG	NE-CZ-NH2	12.74	126.67	120.30
1	D	303	ARG	NE-CZ-NH2	-10.45	115.08	120.30
1	D	303	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	C	303	ARG	CD-NE-CZ	6.34	132.48	123.60
1	D	303	ARG	CD-NE-CZ	5.31	131.03	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	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	3756	0	3538	62	0
1	B	3748	0	3543	50	0
1	C	3764	0	3503	62	0
1	D	3740	0	3444	73	0
2	A	53	0	30	10	0
2	B	53	0	31	5	0
2	C	53	0	30	4	0
2	D	53	0	30	4	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	1	0
4	A	48	0	26	2	0
4	B	48	0	26	1	0
4	C	31	0	11	0	0
4	D	31	0	11	0	0
5	A	8	0	0	0	0
5	B	4	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	1	0
All	All	15449	0	14223	245	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 8.

All (245) 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:D:306:ARG:HH11	1:D:306:ARG:HG2	1.21	1.04
1:A:17:PRO:HD2	2:A:601:FAD:H5'2	1.47	0.96
1:B:453:TYR:CE1	4:B:604:NDP:H42N	2.06	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:PRO:HD2	2:D:601:FAD:H5'2	1.51	0.91
1:A:13:ILE:O	1:A:268:THR:HB	1.78	0.84
1:D:307:PRO:HG2	1:D:310:ILE:HD12	1.59	0.84
1:B:13:ILE:O	1:B:268:THR:HB	1.78	0.83
1:A:245:VAL:HG22	1:A:252:VAL:HG22	1.65	0.78
1:A:453:TYR:CE1	4:A:605:NDP:H42N	2.21	0.76
1:D:306:ARG:NH1	1:D:306:ARG:HG2	1.90	0.75
1:C:125:MET:HE3	1:C:154:ILE:HD12	1.70	0.72
1:D:38:ASP:OD1	2:D:601:FAD:H1B	1.91	0.71
1:A:306:ARG:HB2	1:A:307:PRO:HD2	1.72	0.70
1:B:62:GLY:HA2	1:B:458:GLN:NE2	2.07	0.70
1:C:296:HIS:CE1	1:C:414:ARG:HD2	2.28	0.69
1:C:38:ASP:OD1	2:C:601:FAD:H1B	1.91	0.69
1:D:143:ASP:O	1:D:147:VAL:HG23	1.94	0.68
1:D:296:HIS:CE1	1:D:414:ARG:HD2	2.29	0.68
1:C:13:ILE:O	1:C:268:THR:HB	1.96	0.66
1:D:13:ILE:O	1:D:268:THR:HB	1.95	0.66
1:D:142:PHE:CE1	1:D:179:LEU:HD11	2.31	0.65
1:C:142:PHE:CE1	1:C:179:LEU:HD11	2.31	0.65
1:A:35:MET:CE	1:A:260:ILE:HD13	2.27	0.65
1:A:250:LYS:HG2	1:A:262:TYR:CE1	2.32	0.64
1:D:69:TYR:CG	1:D:463:MET:HG3	2.34	0.63
1:B:306:ARG:HB2	1:B:307:PRO:HD2	1.80	0.62
1:B:46:LEU:HD13	2:B:601:FAD:HM81	1.81	0.61
1:D:69:TYR:CD1	1:D:463:MET:HG3	2.36	0.61
1:C:69:TYR:CG	1:C:463:MET:HG3	2.35	0.61
1:B:250:LYS:HG2	1:B:262:TYR:CE1	2.35	0.60
1:B:313:LYS:HG3	1:B:333:ASN:HB3	1.82	0.60
1:B:37:VAL:HG12	1:B:235:ARG:HB3	1.83	0.60
1:A:62:GLY:HA2	1:A:458:GLN:NE2	2.16	0.59
1:A:130:LEU:HD23	1:D:130:LEU:HD23	1.84	0.59
1:A:69:TYR:CD1	1:A:463:MET:HG3	2.38	0.59
1:B:11:LEU:O	1:B:265:LEU:HD12	2.03	0.59
1:C:79:ALA:HB1	1:C:224:ALA:CB	2.34	0.58
1:D:332:SER:HB3	1:D:369:SER:H	1.68	0.58
1:A:419:TYR:HE2	2:A:601:FAD:HM73	1.69	0.58
1:C:332:SER:HB3	1:C:369:SER:H	1.69	0.58
1:C:92:ILE:HA	1:C:204:TRP:CE3	2.39	0.58
1:C:70:LYS:HE2	1:C:496:ARG:NH2	2.19	0.58
1:D:79:ALA:HB1	1:D:224:ALA:CB	2.34	0.57
1:B:372:LEU:HD21	1:B:395:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ILE:HG22	1:C:94:TYR:HE1	1.70	0.57
1:A:372:LEU:HD21	1:A:395:LEU:HD21	1.86	0.56
1:A:419:TYR:CE2	2:A:601:FAD:HM73	2.39	0.56
1:B:69:TYR:CD1	1:B:463:MET:HG3	2.39	0.56
1:D:306:ARG:HH11	1:D:306:ARG:CG	2.04	0.56
1:B:62:GLY:HA2	1:B:458:GLN:HE22	1.69	0.56
1:C:74:ASP:HB3	1:C:497:LEU:HB2	1.89	0.55
1:A:11:LEU:O	1:A:265:LEU:HD12	2.07	0.55
1:D:192:THR:O	1:D:196:ILE:HG13	2.07	0.55
1:A:21:GLY:HA2	1:A:462:PHE:CE2	2.42	0.54
1:C:332:SER:HB3	1:C:369:SER:N	2.22	0.54
1:B:303:ARG:NH1	1:B:346:LEU:O	2.36	0.54
1:A:192:THR:HG21	1:D:122:ILE:HG21	1.87	0.54
1:D:420:PRO:HD3	1:D:448:PHE:CZ	2.42	0.54
1:D:332:SER:HB3	1:D:369:SER:N	2.22	0.54
1:D:92:ILE:HG22	1:D:94:TYR:HE1	1.72	0.54
1:B:38:ASP:OD1	2:B:601:FAD:H1B	2.08	0.54
1:A:37:VAL:HG12	1:A:235:ARG:HB3	1.90	0.53
1:D:188:LEU:O	1:D:192:THR:HB	2.08	0.53
1:D:27:ASN:HB2	1:D:34:TRP:HZ2	1.73	0.53
1:A:62:GLY:HA2	1:A:458:GLN:HE22	1.72	0.53
1:C:303:ARG:HD2	1:C:406:GLU:OE1	2.08	0.53
1:C:69:TYR:CD1	1:C:463:MET:HG3	2.44	0.53
1:A:69:TYR:CG	1:A:463:MET:HG3	2.43	0.53
1:B:69:TYR:CG	1:B:463:MET:HG3	2.44	0.53
1:A:313:LYS:HG3	1:A:333:ASN:HB3	1.91	0.52
1:D:457:ASN:HB2	2:D:601:FAD:O2	2.08	0.52
1:C:420:PRO:HD3	1:C:448:PHE:CZ	2.45	0.52
1:D:310:ILE:HD13	1:D:368:TRP:CZ3	2.45	0.52
1:A:303:ARG:HD2	1:A:406:GLU:OE1	2.10	0.52
1:C:253:THR:OG1	1:C:259:THR:HG22	2.10	0.52
1:A:35:MET:HE3	1:A:260:ILE:HD13	1.92	0.52
1:A:38:ASP:OD1	2:A:601:FAD:H1B	2.10	0.52
1:C:93:SER:HB3	1:C:315:TRP:NE1	2.26	0.51
1:D:142:PHE:HA	1:D:176:CYS:HB3	1.93	0.51
1:B:457:ASN:HB2	2:B:601:FAD:O2	2.10	0.51
1:B:337:TYR:N	1:B:337:TYR:CD2	2.78	0.51
1:D:92:ILE:HA	1:D:204:TRP:CE3	2.45	0.51
1:B:130:LEU:HD23	1:C:130:LEU:HD23	1.92	0.51
1:D:79:ALA:HB1	1:D:224:ALA:HB1	1.93	0.51
1:C:27:ASN:HB2	1:C:34:TRP:HZ2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TYR:N	1:A:337:TYR:CD2	2.79	0.51
1:C:79:ALA:HB1	1:C:224:ALA:HB1	1.92	0.51
1:D:104:TYR:CG	1:D:105:PRO:HA	2.46	0.50
1:D:204:TRP:HA	1:D:208:ALA:HB3	1.92	0.50
1:B:339:GLN:HB2	1:B:340:PRO:HD2	1.93	0.50
1:D:162:TYR:HB2	1:D:319:PRO:HB3	1.92	0.50
1:C:142:PHE:HA	1:C:176:CYS:HB3	1.93	0.50
1:D:307:PRO:CG	1:D:310:ILE:HD12	2.38	0.50
1:A:334:TYR:N	1:A:334:TYR:CD2	2.80	0.50
1:B:21:GLY:HA2	1:B:462:PHE:CE2	2.46	0.49
1:B:11:LEU:HD13	1:B:35:MET:HE3	1.94	0.49
1:C:104:TYR:CG	1:C:105:PRO:HA	2.47	0.49
1:A:63:HIS:NE2	1:A:334:TYR:HE1	2.11	0.49
1:B:303:ARG:HD2	1:B:406:GLU:OE1	2.13	0.49
1:D:286:LEU:O	1:D:289:GLN:HB2	2.12	0.49
1:D:21:GLY:HA2	1:D:462:PHE:CE2	2.48	0.49
1:D:92:ILE:O	1:D:314:CYS:HB2	2.13	0.49
1:C:188:LEU:O	1:C:192:THR:HB	2.13	0.49
1:B:149:MET:SD	1:B:184:ALA:HA	2.54	0.48
1:B:334:TYR:N	1:B:334:TYR:CD2	2.81	0.48
1:B:265:LEU:HD23	1:B:442:ILE:HG12	1.93	0.48
1:C:212:PHE:CG	1:C:213:PRO:HD2	2.48	0.48
1:D:213:PRO:HG3	1:D:221:ILE:HG13	1.95	0.48
1:A:92:ILE:HG12	1:A:93:SER:H	1.79	0.48
1:C:295:THR:HG21	2:C:601:FAD:C7M	2.44	0.48
1:B:388:LEU:O	1:B:388:LEU:HD12	2.14	0.48
1:B:89:HIS:ND1	1:B:313:LYS:HD3	2.28	0.47
1:C:162:TYR:HB2	1:C:319:PRO:HB3	1.95	0.47
1:A:306:ARG:CB	1:A:307:PRO:HD2	2.37	0.47
1:C:70:LYS:HE2	1:C:496:ARG:HH22	1.79	0.47
1:C:306:ARG:HG3	1:C:306:ARG:O	2.14	0.47
1:A:5:ASP:HB2	1:A:259:THR:O	2.15	0.47
1:B:63:HIS:NE2	1:B:334:TYR:HE1	2.12	0.47
1:B:18:THR:HA	1:B:461:SER:O	2.15	0.47
1:B:359:SER:HB3	1:B:361:GLU:H	1.78	0.47
1:D:93:SER:HB3	1:D:315:TRP:CE2	2.50	0.47
1:A:268:THR:CG2	2:A:601:FAD:H51A	2.44	0.47
1:D:122:ILE:O	1:D:126:ILE:HG13	2.14	0.47
1:A:303:ARG:NH1	1:A:346:LEU:O	2.38	0.47
1:C:461:SER:HA	1:C:464:LEU:HD12	1.95	0.47
1:D:27:ASN:HB2	1:D:34:TRP:CZ2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ASN:HB2	1:C:34:TRP:CZ2	2.50	0.46
2:D:601:FAD:H1'1	2:D:601:FAD:H9	1.48	0.46
1:C:57:LEU:HD12	1:C:57:LEU:N	2.30	0.46
1:D:315:TRP:HE1	1:D:317:TYR:HH	1.62	0.46
1:B:423:THR:HB	1:B:425:GLU:OE1	2.15	0.46
1:C:87:TYR:HE2	1:C:214:ALA:HB1	1.80	0.46
1:D:334:TYR:N	1:D:334:TYR:CD2	2.84	0.46
1:A:143:ASP:O	1:A:147:VAL:HG23	2.15	0.46
1:A:292:TYR:CZ	1:A:417:HIS:CE1	3.04	0.46
1:C:306:ARG:HA	1:C:307:PRO:HD2	1.61	0.46
1:C:337:TYR:N	1:C:337:TYR:CD2	2.84	0.46
1:D:337:TYR:N	1:D:337:TYR:CD2	2.83	0.46
1:A:339:GLN:HB2	1:A:340:PRO:HD2	1.98	0.46
1:C:104:TYR:HD1	1:C:203:ASN:ND2	2.13	0.45
1:A:29:ILE:HG22	1:A:31:GLY:N	2.32	0.45
1:A:431:THR:O	1:A:435:PRO:HG2	2.17	0.45
1:B:92:ILE:O	1:B:314:CYS:HB2	2.15	0.45
1:B:426:ARG:O	1:B:430:LEU:HB2	2.16	0.45
1:C:445:ARG:NE	1:C:481:LEU:HD22	2.31	0.45
1:D:310:ILE:CD1	1:D:368:TRP:CZ3	3.00	0.45
1:A:345:ALA:HA	1:A:363:LYS:O	2.17	0.45
1:C:205:GLY:N	1:C:208:ALA:HB3	2.32	0.45
1:A:334:TYR:N	1:A:334:TYR:HD2	2.15	0.45
1:A:423:THR:HB	1:A:425:GLU:OE1	2.17	0.45
1:D:125:MET:HE3	1:D:154:ILE:HD12	1.99	0.45
1:D:212:PHE:CD1	1:D:213:PRO:HD2	2.52	0.45
1:D:250:LYS:HG2	1:D:262:TYR:CE1	2.52	0.44
1:D:461:SER:HA	1:D:464:LEU:HD12	1.98	0.44
1:C:69:TYR:CD2	1:C:463:MET:HG3	2.52	0.44
1:B:27:ASN:HB2	1:B:34:TRP:CZ2	2.53	0.44
1:D:57:LEU:HD12	1:D:57:LEU:N	2.32	0.44
1:B:504:PHE:CD2	1:D:32:PRO:HB3	2.53	0.44
1:D:80:LEU:HD12	1:D:86:TRP:CZ2	2.52	0.44
1:A:265:LEU:HD23	1:A:442:ILE:HG12	1.98	0.44
1:D:11:LEU:HD13	1:D:260:ILE:HG21	2.00	0.44
1:D:310:ILE:HG21	1:D:330:ILE:HD12	1.98	0.44
1:D:421:THR:HA	1:D:422:PRO:HD3	1.84	0.44
1:D:434:LEU:HB2	1:D:435:PRO:HD3	2.00	0.44
1:A:307:PRO:HD3	1:A:368:TRP:CH2	2.53	0.44
1:B:334:TYR:N	1:B:334:TYR:HD2	2.15	0.44
1:C:280:ASP:O	1:C:284:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:SER:HA	1:D:219:GLY:HA3	1.99	0.44
1:A:350:GLN:HG3	1:A:351:LEU:O	2.18	0.44
1:C:197:LEU:HA	1:C:197:LEU:HD23	1.81	0.44
1:C:421:THR:HA	1:C:422:PRO:HD3	1.84	0.44
1:A:11:LEU:HD13	1:A:35:MET:HE3	2.00	0.43
1:D:303:ARG:HD3	1:D:364:GLU:O	2.17	0.43
1:B:125:MET:SD	1:B:191:VAL:HG21	2.58	0.43
1:C:17:PRO:HD2	2:C:601:FAD:O1P	2.17	0.43
2:B:601:FAD:H9	2:B:601:FAD:H1'1	1.61	0.43
1:C:65:ILE:CG2	1:C:66:PHE:N	2.81	0.43
1:C:87:TYR:CE2	1:C:214:ALA:CB	3.02	0.43
1:A:27:ASN:HB2	1:A:34:TRP:CZ2	2.53	0.43
2:C:601:FAD:N1	2:C:601:FAD:H2'	2.33	0.43
1:A:35:MET:HE1	1:A:260:ILE:HD13	2.00	0.43
1:D:412:HIS:CD2	1:D:412:HIS:C	2.90	0.43
1:B:292:TYR:CZ	1:B:417:HIS:CE1	3.06	0.43
1:C:113:LEU:HB3	1:C:114:PRO:HD2	1.99	0.43
1:A:102:VAL:HA	1:A:103:PRO:HD3	1.81	0.43
1:B:342:ALA:HB2	1:B:366:PRO:HB3	2.00	0.43
1:A:412:HIS:C	1:A:412:HIS:CD2	2.91	0.42
1:A:458:GLN:HG3	2:A:601:FAD:N1	2.35	0.42
1:A:65:ILE:HD12	1:A:91:ARG:HD3	2.01	0.42
1:B:142:PHE:CE1	1:B:179:LEU:HD11	2.54	0.42
1:B:29:ILE:HG22	1:B:31:GLY:N	2.34	0.42
1:D:125:MET:CE	1:D:154:ILE:HD12	2.48	0.42
2:A:601:FAD:O2'	2:A:601:FAD:H9	2.19	0.42
1:B:339:GLN:HB2	1:B:340:PRO:CD	2.49	0.42
1:C:434:LEU:HB2	1:C:435:PRO:HD3	2.01	0.42
1:C:92:ILE:HD13	1:C:312:ASP:OD1	2.20	0.42
1:D:104:TYR:O	1:D:202:GLY:HA2	2.19	0.42
1:D:430:LEU:HD12	1:D:430:LEU:HA	1.84	0.42
1:B:215:ARG:NH1	1:B:337:TYR:CE1	2.88	0.42
1:C:380:LYS:HG2	1:C:380:LYS:O	2.19	0.42
1:D:292:TYR:CZ	1:D:417:HIS:CE1	3.08	0.42
1:A:302:VAL:HG12	1:A:303:ARG:N	2.34	0.42
1:A:334:TYR:H	1:A:334:TYR:HD2	1.66	0.42
1:C:414:ARG:HH11	1:C:414:ARG:HG2	1.84	0.42
1:D:192:THR:CG2	5:D:701:HOH:O	2.66	0.42
1:A:342:ALA:HB2	1:A:366:PRO:HB3	2.01	0.42
1:B:326:TYR:CZ	1:B:373:GLU:HB3	2.55	0.42
1:D:280:ASP:O	1:D:284:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:ASN:OD1	1:D:460:HIS:ND1	2.53	0.42
1:C:412:HIS:CD2	1:C:412:HIS:C	2.93	0.42
1:C:9:ASP:OD1	1:C:263:LYS:HE3	2.20	0.42
1:D:334:TYR:HD2	1:D:334:TYR:N	2.16	0.42
1:A:145:TRP:CD2	1:A:179:LEU:HD13	2.55	0.42
1:A:149:MET:SD	1:A:184:ALA:HA	2.59	0.42
1:A:339:GLN:HB2	1:A:340:PRO:CD	2.50	0.42
1:B:5:ASP:HB2	1:B:259:THR:O	2.19	0.42
1:C:21:GLY:HA2	1:C:462:PHE:CE2	2.55	0.42
1:B:295:THR:HG21	2:B:601:FAD:C7M	2.50	0.41
1:D:113:LEU:HB3	1:D:114:PRO:HD2	2.01	0.41
1:D:69:TYR:CD2	1:D:463:MET:HG3	2.55	0.41
1:C:430:LEU:HA	1:C:430:LEU:HD12	1.86	0.41
1:A:457:ASN:HB2	2:A:601:FAD:C2	2.50	0.41
1:D:47:ALA:O	1:D:218:THR:HG22	2.20	0.41
1:C:48:SER:HA	1:C:219:GLY:HA3	2.02	0.41
1:C:213:PRO:HG3	1:C:221:ILE:HG13	2.01	0.41
1:D:445:ARG:NE	1:D:481:LEU:HD22	2.35	0.41
1:C:122:ILE:O	1:C:126:ILE:HG13	2.21	0.41
1:C:334:TYR:N	1:C:334:TYR:CD2	2.88	0.41
1:D:487:VAL:HG23	1:D:488:ASN:N	2.35	0.41
1:A:457:ASN:ND2	4:A:605:NDP:C6N	2.84	0.41
1:C:175:GLN:O	1:C:178:TRP:NE1	2.53	0.41
1:A:17:PRO:CD	2:A:601:FAD:H5'2	2.34	0.41
1:D:453:TYR:CE1	3:D:604:SO4:O2	2.74	0.41
1:A:326:TYR:CZ	1:A:373:GLU:HB3	2.55	0.41
1:B:122:ILE:HG13	1:C:196:ILE:HD11	2.02	0.41
1:B:59:ASP:HB3	1:B:62:GLY:H	1.86	0.41
1:C:457:ASN:OD1	1:C:460:HIS:ND1	2.54	0.41
1:B:472:ILE:O	1:D:500:GLY:HA3	2.21	0.41
1:A:487:VAL:HG23	1:A:488:ASN:N	2.36	0.40
1:D:337:TYR:N	1:D:337:TYR:HD2	2.20	0.40
1:A:18:THR:HA	1:A:461:SER:O	2.20	0.40
1:B:192:THR:O	1:B:196:ILE:HG13	2.20	0.40
1:C:250:LYS:HG2	1:C:262:TYR:CE1	2.57	0.40
1:D:104:TYR:HD1	1:D:203:ASN:HD21	1.69	0.40
1:A:46:LEU:HD13	2:A:601:FAD:HM81	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	491/513 (96%)	472 (96%)	19 (4%)	0	100	100
1	B	486/513 (95%)	464 (96%)	22 (4%)	0	100	100
1	C	497/513 (97%)	468 (94%)	29 (6%)	0	100	100
1	D	493/513 (96%)	467 (95%)	26 (5%)	0	100	100
All	All	1967/2052 (96%)	1871 (95%)	96 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/432 (88%)	370 (98%)	8 (2%)	61	88
1	B	383/432 (89%)	371 (97%)	12 (3%)	47	79
1	C	376/432 (87%)	360 (96%)	16 (4%)	35	68
1	D	368/432 (85%)	353 (96%)	15 (4%)	37	69
All	All	1505/1728 (87%)	1454 (97%)	51 (3%)	44	76

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	MET
1	A	159	MET

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Mol	Chain	Res	Type
1	A	169	VAL
1	A	251	THR
1	A	252	VAL
1	A	268	THR
1	A	470	ASP
1	A	485	ASP
1	B	64	VAL
1	B	149	MET
1	B	159	MET
1	B	169	VAL
1	B	251	THR
1	B	268	THR
1	B	306	ARG
1	B	313	LYS
1	B	359	SER
1	B	426	ARG
1	B	470	ASP
1	B	485	ASP
1	C	27	ASN
1	C	149	MET
1	C	159	MET
1	C	175	GLN
1	C	192	THR
1	C	200	THR
1	C	218	THR
1	C	267	SER
1	C	268	THR
1	C	305	SER
1	C	337	TYR
1	C	377	SER
1	C	378	SER
1	C	430	LEU
1	C	470	ASP
1	C	485	ASP
1	D	147	VAL
1	D	149	MET
1	D	159	MET
1	D	175	GLN
1	D	192	THR
1	D	218	THR
1	D	267	SER
1	D	268	THR

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Mol	Chain	Res	Type
1	D	306	ARG
1	D	337	TYR
1	D	377	SER
1	D	378	SER
1	D	430	LEU
1	D	470	ASP
1	D	485	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	B	98	GLN
1	D	98	GLN

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](#)

19 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	-	52,58,58	1.96	17 (32%)	52,89,89	2.67	19 (36%)
3	SO4	A	602	-	4,4,4	0.13	0	6,6,6	0.20	0
3	SO4	A	603	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	A	604	-	4,4,4	0.21	0	6,6,6	0.43	0
4	NDP	A	605	-	44,52,52	1.69	11 (25%)	55,80,80	2.14	11 (20%)
2	FAD	B	601	-	52,58,58	1.98	21 (40%)	52,89,89	2.61	17 (32%)
3	SO4	B	602	-	4,4,4	0.18	0	6,6,6	0.27	0
3	SO4	B	603	-	4,4,4	0.23	0	6,6,6	0.31	0
4	NDP	B	604	-	44,52,52	1.69	12 (27%)	55,80,80	2.15	8 (14%)
2	FAD	C	601	-	52,58,58	1.98	17 (32%)	52,89,89	2.39	16 (30%)
3	SO4	C	602	-	4,4,4	0.20	0	6,6,6	0.34	0
3	SO4	C	603	-	4,4,4	0.19	0	6,6,6	0.12	0
3	SO4	C	604	-	4,4,4	0.25	0	6,6,6	0.12	0
4	NDP	C	605	-	27,33,52	1.45	5 (18%)	32,52,80	2.30	4 (12%)
2	FAD	D	601	-	52,58,58	2.06	18 (34%)	52,89,89	2.57	15 (28%)
3	SO4	D	602	-	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	D	603	-	4,4,4	0.29	0	6,6,6	0.26	0
3	SO4	D	604	-	4,4,4	0.33	0	6,6,6	0.27	0
4	NDP	D	605	-	27,33,52	1.47	5 (18%)	32,52,80	2.33	5 (15%)

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	-	-	0/30/50/50	0/6/6/6
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	A	604	-	-	0/0/0/0	0/0/0/0
4	NDP	A	605	-	-	0/30/77/77	0/5/5/5
2	FAD	B	601	-	-	0/30/50/50	0/6/6/6
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	SO4	B	603	-	-	0/0/0/0	0/0/0/0
4	NDP	B	604	-	-	0/30/77/77	0/5/5/5
2	FAD	C	601	-	-	0/30/50/50	0/6/6/6
3	SO4	C	602	-	-	0/0/0/0	0/0/0/0
3	SO4	C	603	-	-	0/0/0/0	0/0/0/0
3	SO4	C	604	-	-	0/0/0/0	0/0/0/0
4	NDP	C	605	-	-	0/17/37/77	0/3/3/5
2	FAD	D	601	-	-	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	D	602	-	-	0/0/0/0	0/0/0/0
3	SO4	D	603	-	-	0/0/0/0	0/0/0/0
3	SO4	D	604	-	-	0/0/0/0	0/0/0/0
4	NDP	D	605	-	-	0/17/37/77	0/3/3/5

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	O2'-C2'	-3.59	1.35	1.43
4	A	605	NDP	C4N-C5N	-3.40	1.41	1.49
2	C	601	FAD	C2B-C1B	-3.30	1.48	1.53
2	B	601	FAD	C2B-C1B	-3.22	1.48	1.53
2	B	601	FAD	C1'-N10	-3.16	1.45	1.48
2	A	601	FAD	C2B-C1B	-3.13	1.48	1.53
4	B	604	NDP	C4N-C5N	-3.08	1.42	1.49
2	C	601	FAD	O2'-C2'	-2.95	1.36	1.43
2	D	601	FAD	O2'-C2'	-2.93	1.36	1.43
2	D	601	FAD	C2B-C1B	-2.91	1.49	1.53
2	C	601	FAD	O4'-C4'	-2.90	1.36	1.43
2	D	601	FAD	O4'-C4'	-2.89	1.36	1.43
2	C	601	FAD	PA-O5B	-2.89	1.46	1.59
2	B	601	FAD	O2'-C2'	-2.86	1.37	1.43
2	D	601	FAD	PA-O5B	-2.81	1.47	1.59
2	B	601	FAD	PA-O5B	-2.78	1.47	1.59
2	A	601	FAD	O4'-C4'	-2.71	1.37	1.43
2	B	601	FAD	O4'-C4'	-2.66	1.37	1.43
4	D	605	NDP	PA-O5B	-2.65	1.47	1.59
2	D	601	FAD	PA-O2A	-2.63	1.43	1.55
2	A	601	FAD	PA-O2A	-2.62	1.44	1.55
2	A	601	FAD	PA-O5B	-2.62	1.48	1.59
4	B	604	NDP	PA-O2A	-2.55	1.44	1.55
4	C	605	NDP	PA-O5B	-2.54	1.48	1.59
4	B	604	NDP	C3B-C2B	-2.53	1.47	1.53
4	D	605	NDP	PA-O2A	-2.52	1.44	1.55
2	B	601	FAD	C4'-C3'	-2.45	1.48	1.53
4	A	605	NDP	C3B-C2B	-2.45	1.47	1.53
2	C	601	FAD	PA-O2A	-2.44	1.44	1.55
4	A	605	NDP	O2D-C2D	-2.41	1.37	1.43
2	B	601	FAD	O3'-C3'	-2.38	1.37	1.43
4	C	605	NDP	PA-O2A	-2.37	1.45	1.55
2	A	601	FAD	O3'-C3'	-2.34	1.37	1.43
2	B	601	FAD	PA-O2A	-2.33	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C2B-C3B	-2.33	1.47	1.53
4	A	605	NDP	PA-O2A	-2.31	1.45	1.55
4	A	605	NDP	PA-O5B	-2.25	1.49	1.59
2	C	601	FAD	C1'-N10	-2.25	1.46	1.48
4	B	604	NDP	PA-O5B	-2.25	1.49	1.59
2	C	601	FAD	O2B-C2B	-2.23	1.37	1.43
4	D	605	NDP	C3B-C2B	-2.23	1.48	1.53
2	A	601	FAD	C2B-C3B	-2.21	1.47	1.53
2	A	601	FAD	O2B-C2B	-2.17	1.37	1.43
4	B	604	NDP	O2D-C2D	-2.16	1.37	1.43
2	D	601	FAD	C2B-C3B	-2.16	1.47	1.53
2	C	601	FAD	C2B-C3B	-2.14	1.47	1.53
2	A	601	FAD	C4'-C3'	-2.10	1.49	1.53
2	C	601	FAD	O3'-C3'	-2.09	1.38	1.43
4	C	605	NDP	O3B-C3B	-2.08	1.38	1.43
2	B	601	FAD	O4B-C4B	-2.06	1.40	1.45
2	D	601	FAD	O3B-C3B	-2.05	1.38	1.43
2	B	601	FAD	O2B-C2B	-2.00	1.38	1.43
4	B	604	NDP	C2N-C3N	2.02	1.40	1.34
2	C	601	FAD	C5X-N5	2.02	1.38	1.35
2	B	601	FAD	C4X-C10	2.04	1.44	1.40
4	A	605	NDP	C2N-C3N	2.06	1.40	1.34
4	A	605	NDP	C6N-N1N	2.15	1.42	1.37
4	B	604	NDP	C2N-N1N	2.20	1.41	1.37
2	D	601	FAD	C10-N10	2.28	1.41	1.39
4	B	604	NDP	C2A-N3A	2.30	1.36	1.32
2	B	601	FAD	C6A-N6A	2.34	1.43	1.34
4	B	604	NDP	C6N-N1N	2.39	1.43	1.37
2	B	601	FAD	C2A-N3A	2.43	1.36	1.32
2	A	601	FAD	C6A-N6A	2.45	1.44	1.34
2	A	601	FAD	C9A-N10	2.45	1.42	1.38
2	B	601	FAD	C5X-N5	2.46	1.39	1.35
2	B	601	FAD	P-O1P	2.46	1.60	1.51
2	C	601	FAD	C2A-N3A	2.47	1.36	1.32
4	C	605	NDP	C2A-N3A	2.52	1.36	1.32
2	D	601	FAD	P-O1P	2.53	1.60	1.51
4	D	605	NDP	C6A-N6A	2.54	1.44	1.34
2	D	601	FAD	C4X-C10	2.55	1.45	1.40
2	C	601	FAD	C6A-N6A	2.55	1.44	1.34
2	A	601	FAD	C2-N1	2.56	1.43	1.38
2	A	601	FAD	C2A-N3A	2.56	1.36	1.32
2	D	601	FAD	C5X-N5	2.57	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	NDP	C2A-N3A	2.57	1.36	1.32
2	D	601	FAD	C2A-N3A	2.59	1.36	1.32
4	D	605	NDP	C2A-N3A	2.59	1.36	1.32
4	C	605	NDP	C6A-N6A	2.64	1.45	1.34
2	D	601	FAD	C6A-N6A	2.66	1.45	1.34
4	B	604	NDP	C6A-N6A	2.66	1.45	1.34
4	A	605	NDP	C6A-N6A	2.66	1.45	1.34
2	B	601	FAD	C2-N1	2.66	1.43	1.38
2	D	601	FAD	C2-N1	2.71	1.43	1.38
2	A	601	FAD	C4X-N5	2.90	1.37	1.33
2	C	601	FAD	C2-N1	2.97	1.44	1.38
2	C	601	FAD	C4-N3	3.12	1.38	1.33
2	B	601	FAD	C4-C4X	3.34	1.48	1.41
4	A	605	NDP	C7N-N7N	3.46	1.43	1.33
2	D	601	FAD	C4X-N5	3.47	1.38	1.33
4	B	604	NDP	C7N-N7N	3.60	1.43	1.33
2	A	601	FAD	C4-C4X	3.66	1.48	1.41
2	D	601	FAD	C4-N3	3.68	1.39	1.33
2	C	601	FAD	C4X-N5	3.69	1.39	1.33
2	B	601	FAD	C4-N3	3.79	1.39	1.33
2	B	601	FAD	C4X-N5	3.98	1.39	1.33
4	B	604	NDP	C6N-C5N	4.00	1.40	1.33
2	A	601	FAD	C4-N3	4.05	1.40	1.33
4	A	605	NDP	C6N-C5N	4.10	1.40	1.33
2	C	601	FAD	C4-C4X	4.45	1.50	1.41
2	D	601	FAD	C4-C4X	5.14	1.51	1.41
2	C	601	FAD	O4-C4	5.40	1.38	1.24
2	A	601	FAD	O4-C4	5.45	1.38	1.24
2	B	601	FAD	O4-C4	5.47	1.38	1.24
2	D	601	FAD	O4-C4	5.81	1.39	1.24

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	NDP	N3A-C2A-N1A	-11.73	119.66	128.87
4	B	604	NDP	N3A-C2A-N1A	-11.62	119.75	128.87
2	A	601	FAD	N3A-C2A-N1A	-11.53	119.81	128.87
2	B	601	FAD	N3A-C2A-N1A	-11.39	119.92	128.87
4	D	605	NDP	N3A-C2A-N1A	-10.68	120.48	128.87
4	C	605	NDP	N3A-C2A-N1A	-10.64	120.51	128.87
2	D	601	FAD	N3A-C2A-N1A	-10.27	120.80	128.87
2	C	601	FAD	N3A-C2A-N1A	-9.92	121.08	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4B-O4B-C1B	-5.82	103.47	109.64
2	A	601	FAD	N3-C2-N1	-4.42	120.25	127.69
2	B	601	FAD	N3-C2-N1	-4.11	120.77	127.69
2	C	601	FAD	N3-C2-N1	-4.10	120.78	127.69
2	D	601	FAD	O2A-PA-O3P	-4.08	87.78	105.27
2	D	601	FAD	O2P-P-O3P	-4.03	88.01	105.27
2	B	601	FAD	O2A-PA-O3P	-4.02	88.02	105.27
2	D	601	FAD	C4X-C4-N3	-3.92	118.40	123.52
2	D	601	FAD	N3-C2-N1	-3.79	121.32	127.69
2	D	601	FAD	C1'-N10-C9A	-3.75	114.48	118.83
2	B	601	FAD	C4-C4X-C10	-3.51	117.69	119.94
2	C	601	FAD	C1'-N10-C9A	-3.46	114.82	118.83
4	D	605	NDP	C1B-N9A-C4A	-3.40	123.01	126.81
2	A	601	FAD	O2P-P-O3P	-3.24	91.39	105.27
2	B	601	FAD	C4X-C4-N3	-3.16	119.39	123.52
2	A	601	FAD	O2A-PA-O3P	-3.04	92.23	105.27
4	D	605	NDP	O2A-PA-O5B	-2.98	94.05	108.24
2	C	601	FAD	C4X-C4-N3	-2.94	119.68	123.52
4	B	604	NDP	O2A-PA-O3	-2.94	92.68	105.27
2	C	601	FAD	O2P-P-O3P	-2.89	92.88	105.27
4	C	605	NDP	O2A-PA-O5B	-2.87	94.57	108.24
2	A	601	FAD	C4X-C4-N3	-2.86	119.79	123.52
2	B	601	FAD	C4X-C10-N10	-2.63	118.61	120.52
4	B	604	NDP	C3N-C2N-N1N	-2.61	119.41	123.24
2	C	601	FAD	O2A-PA-O5B	-2.61	95.81	108.24
4	A	605	NDP	O2A-PA-O3	-2.59	94.15	105.27
2	C	601	FAD	C4-C4X-C10	-2.55	118.31	119.94
4	A	605	NDP	C4B-O4B-C1B	-2.52	106.97	109.64
2	B	601	FAD	O2P-P-O3P	-2.52	94.46	105.27
2	C	601	FAD	O2P-P-O5'	-2.52	96.25	108.24
2	C	601	FAD	C4X-C10-N10	-2.50	118.70	120.52
2	A	601	FAD	C4-C4X-C10	-2.46	118.37	119.94
2	D	601	FAD	O2A-PA-O5B	-2.46	96.53	108.24
2	A	601	FAD	O2P-P-O5'	-2.44	96.60	108.24
4	A	605	NDP	C3N-C2N-N1N	-2.40	119.71	123.24
4	B	604	NDP	C4B-O4B-C1B	-2.39	107.11	109.64
2	A	601	FAD	O2A-PA-O5B	-2.36	96.98	108.24
4	A	605	NDP	C4D-O4D-C1D	-2.27	104.52	109.52
2	A	601	FAD	C4X-C10-N10	-2.26	118.87	120.52
2	B	601	FAD	O2A-PA-O5B	-2.22	97.64	108.24
2	B	601	FAD	C1'-C2'-C3'	-2.22	103.46	109.82
4	A	605	NDP	O2A-PA-O5B	-2.21	97.72	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	604	NDP	C1B-N9A-C4A	-2.19	124.36	126.81
2	D	601	FAD	O2P-P-O5'	-2.13	98.08	108.24
4	A	605	NDP	C1D-N1N-C2N	-2.07	117.25	120.85
2	D	601	FAD	C4-C4X-C10	-2.04	118.63	119.94
2	A	601	FAD	C1'-N10-C9A	2.08	121.24	118.83
4	D	605	NDP	O4B-C1B-N9A	2.09	112.05	108.11
2	A	601	FAD	O5B-C5B-C4B	2.10	116.67	109.09
4	A	605	NDP	O5B-PA-O1A	2.11	117.86	109.21
2	C	601	FAD	O5'-P-O1P	2.21	118.25	109.21
2	B	601	FAD	C4X-N5-C5X	2.23	119.35	116.72
2	B	601	FAD	C4-C4X-N5	2.33	121.53	118.70
4	D	605	NDP	O5B-PA-O1A	2.34	118.77	109.21
4	A	605	NDP	C5N-C4N-C3N	2.35	118.49	112.41
2	A	601	FAD	O4'-C4'-C5'	2.47	115.49	110.09
4	C	605	NDP	O5B-PA-O1A	2.56	119.69	109.21
2	A	601	FAD	C4-C4X-N5	2.61	121.87	118.70
2	B	601	FAD	O3'-C3'-C2'	2.64	115.57	108.73
2	C	601	FAD	O5B-PA-O1A	2.70	120.28	109.21
2	A	601	FAD	O5B-PA-O1A	2.72	120.37	109.21
2	A	601	FAD	O5'-P-O1P	2.74	120.45	109.21
4	A	605	NDP	O4B-C1B-N9A	2.76	113.33	108.11
4	B	604	NDP	C5N-C4N-C3N	2.90	119.93	112.41
2	D	601	FAD	O5B-PA-O1A	2.94	121.25	109.21
2	B	601	FAD	O5B-PA-O1A	2.97	121.35	109.21
2	C	601	FAD	C5X-C9A-N10	3.08	119.89	117.58
2	B	601	FAD	O5'-P-O1P	3.13	122.03	109.21
2	C	601	FAD	C4-C4X-N5	3.14	122.52	118.70
2	C	601	FAD	O4B-C1B-N9A	3.17	114.10	108.11
4	C	605	NDP	O4B-C1B-N9A	3.19	114.12	108.11
4	B	604	NDP	O2B-P2B-O1X	3.21	115.13	107.48
2	D	601	FAD	O5'-P-O1P	3.22	122.39	109.21
2	D	601	FAD	C5X-C9A-N10	3.55	120.24	117.58
2	A	601	FAD	C4X-N5-C5X	3.75	121.14	116.72
2	B	601	FAD	O4B-C1B-N9A	3.76	115.20	108.11
2	D	601	FAD	C4-C4X-N5	3.89	123.42	118.70
2	B	601	FAD	C5X-C9A-N10	4.01	120.58	117.58
2	C	601	FAD	C4X-N5-C5X	4.02	121.46	116.72
2	D	601	FAD	C4X-N5-C5X	4.32	121.81	116.72
4	A	605	NDP	O4D-C1D-N1N	4.72	117.09	108.09
2	A	601	FAD	O4B-C1B-N9A	4.72	117.03	108.11
4	B	604	NDP	O4D-C1D-N1N	5.20	118.00	108.09
2	A	601	FAD	C4-N3-C2	5.98	120.15	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	601	FAD	C4-N3-C2	6.20	120.33	115.16
2	B	601	FAD	C4-N3-C2	6.56	120.63	115.16
2	D	601	FAD	C4-N3-C2	6.93	120.94	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	10	0
4	A	605	NDP	2	0
2	B	601	FAD	5	0
4	B	604	NDP	1	0
2	C	601	FAD	4	0
2	D	601	FAD	4	0
3	D	604	SO4	1	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	495/513 (96%)	0.21	1 (0%) 95 95	25, 47, 79, 107	0
1	B	492/513 (95%)	0.18	0 100 100	26, 47, 79, 112	0
1	C	501/513 (97%)	0.32	6 (1%) 81 76	21, 56, 89, 110	0
1	D	499/513 (97%)	0.33	8 (1%) 74 70	23, 56, 91, 109	0
All	All	1987/2052 (96%)	0.26	15 (0%) 87 83	21, 51, 85, 112	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	236	PHE	3.4
1	D	225	VAL	3.2
1	D	36	ILE	3.2
1	D	204	TRP	3.0
1	D	37	VAL	3.0
1	D	504	PHE	2.9
1	D	242	VAL	2.8
1	C	12	VAL	2.5
1	C	11	LEU	2.4
1	C	254	LEU	2.3
1	A	504	PHE	2.2
1	C	236	PHE	2.1
1	C	203	ASN	2.1
1	D	44	GLY	2.0
1	C	64	VAL	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
3	SO4	C	604	5/5	0.93	0.40	4.89	86,91,108,109	5
3	SO4	D	604	5/5	0.97	0.28	1.67	63,81,88,91	5
4	NDP	D	605	31/48	0.93	0.23	0.44	21,71,109,110	31
4	NDP	B	604	48/48	0.98	0.20	0.36	17,47,61,78	0
2	FAD	A	601	53/53	0.98	0.22	0.14	16,40,59,74	0
2	FAD	B	601	53/53	0.98	0.19	0.03	20,39,56,69	0
2	FAD	D	601	53/53	0.97	0.20	-0.54	25,63,86,100	0
2	FAD	C	601	53/53	0.98	0.20	-0.56	30,60,83,107	0
3	SO4	B	603	5/5	0.97	0.18	-1.10	63,67,70,85	0
4	NDP	C	605	31/48	0.93	0.18	-1.18	20,59,86,88	31
4	NDP	A	605	48/48	0.97	0.18	-1.45	27,51,72,78	0
3	SO4	A	602	5/5	0.96	0.16	-	31,44,93,95	5
3	SO4	D	602	5/5	0.95	0.15	-	49,63,80,87	5
3	SO4	B	602	5/5	0.96	0.12	-	40,64,98,107	5
3	SO4	A	604	5/5	0.97	0.16	-	57,57,74,77	0
3	SO4	A	603	5/5	0.96	0.12	-	60,80,95,106	5
3	SO4	D	603	5/5	0.95	0.16	-	64,67,93,96	5
3	SO4	C	603	5/5	0.94	0.25	-	46,93,101,103	5
3	SO4	C	602	5/5	0.95	0.18	-	45,48,81,113	5

6.5 Other polymers [i](#)

There are no such residues in this entry.