



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:51 PM GMT

PDB ID : 4YRY  
Title : Insights into flavin-based electron bifurcation via the NADH-dependent reduced ferredoxin-NADP oxidoreductase structure  
Authors : Ermler, U.; Thauer, R.K.; Demmer, J.K.; Huang, H.; Wang, S.; Demmer, U.  
Deposited on : 2015-03-16  
Resolution : 2.40 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](mailto: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.

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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-20026982  
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-20026982

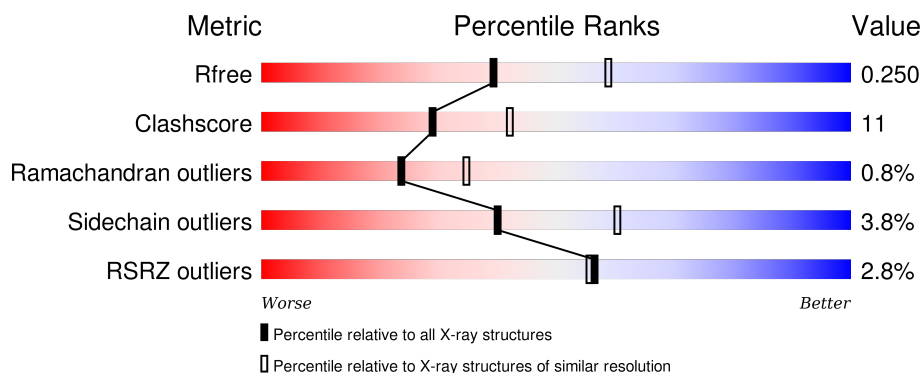
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	276	<div> <div>2%</div> <div>64% 32%</div> <div>•</div> </div>
1	C	276	<div> <div>8%</div> <div>65% 28%</div> <div>• •</div> </div>
2	B	468	<div> <div>2%</div> <div>71% 29%</div> <div>•</div> </div>
2	D	468	<div> <div>2%</div> <div>78% 21%</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	SF4	B	501	-	-	-	X
6	SF4	B	502	-	-	-	X
6	SF4	D	501	-	-	-	X
6	SF4	D	502	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11916 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.

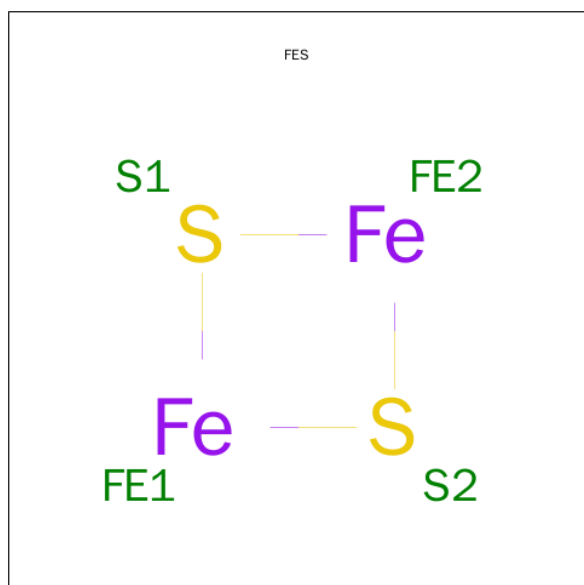
- Molecule 1 is a protein called Dihydroorotate dehydrogenase B (NAD(+)), electron transfer subunit homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2140	1369	359	398	14			
1	C	265	Total	C	N	O	S	0	0	0
			2049	1310	343	383	13			

- Molecule 2 is a protein called Dihydropyrimidine dehydrogenase subunit A.

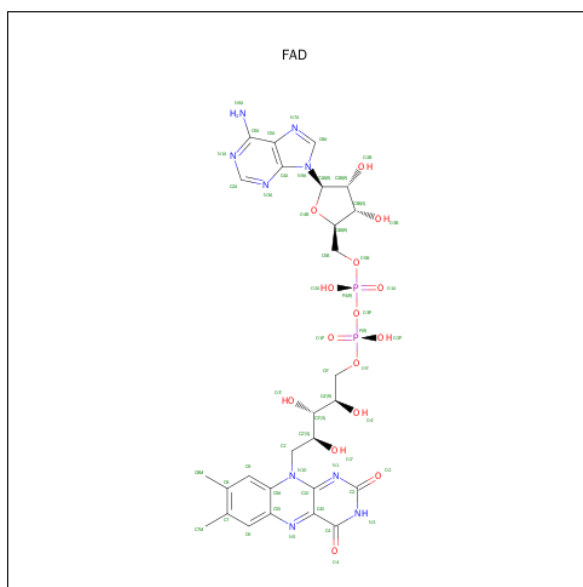
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	468	Total	C	N	O	S	0	0	0
			3625	2295	636	673	21			
2	D	468	Total	C	N	O	S	0	0	0
			3625	2295	636	673	21			

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



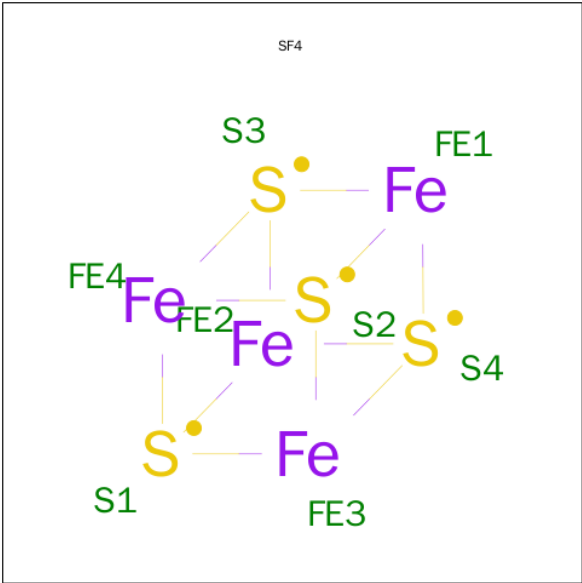
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



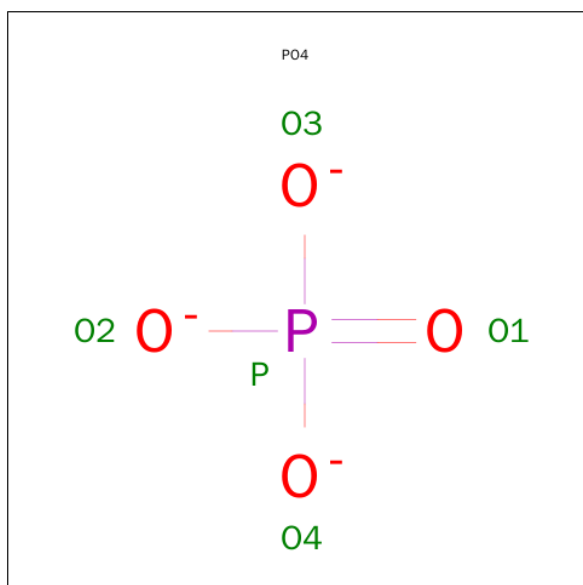
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	Fe	S	0	0
			8	4	4		
6	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	O	P	0	0
			5	4	1		

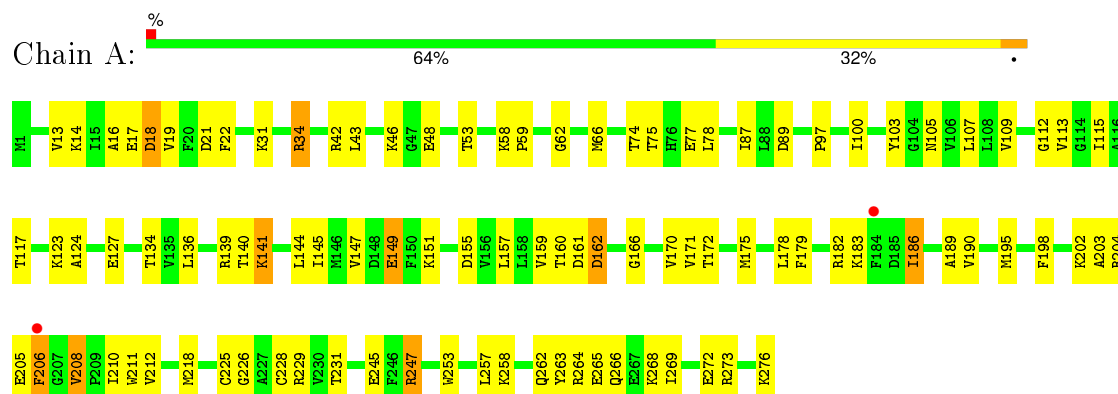
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	15	Total	O	0	0
			15	15		
8	B	56	Total	O	0	0
			56	56		
8	C	20	Total	O	0	0
			20	20		
8	D	41	Total	O	0	0
			41	41		

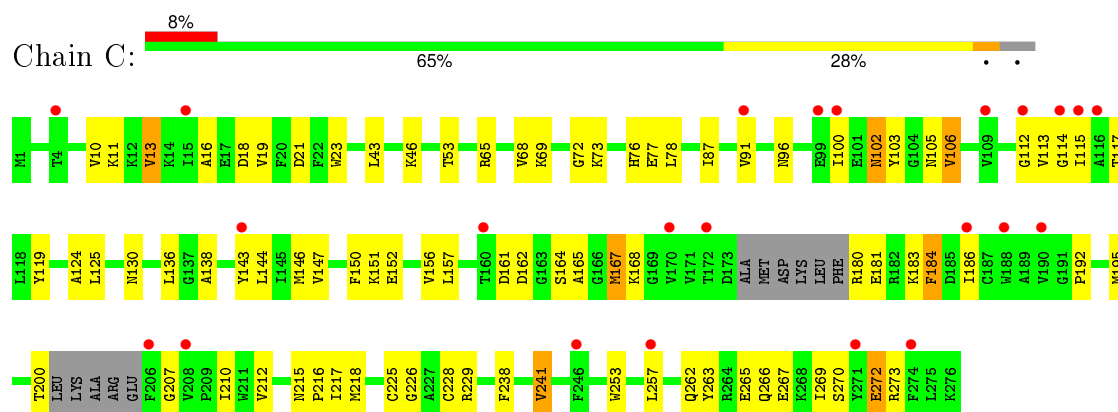
### 3 Residue-property plots

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.

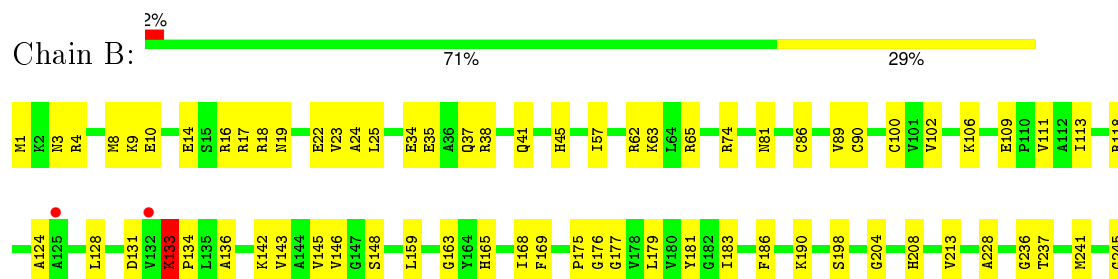
- Molecule 1: Dihydroorotate dehydrogenase B (NAD(+)), electron transfer subunit homolog



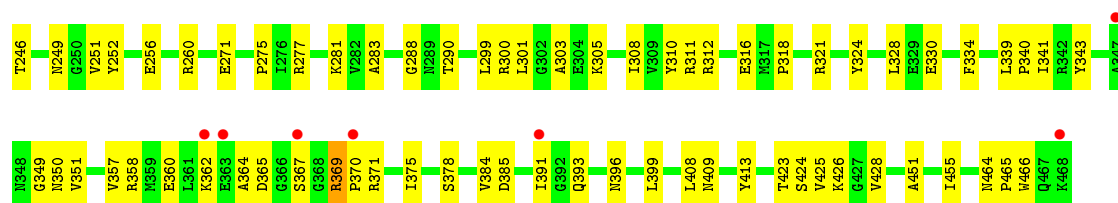
- Molecule 1: Dihydroorotate dehydrogenase B (NAD(+)), electron transfer subunit homolog



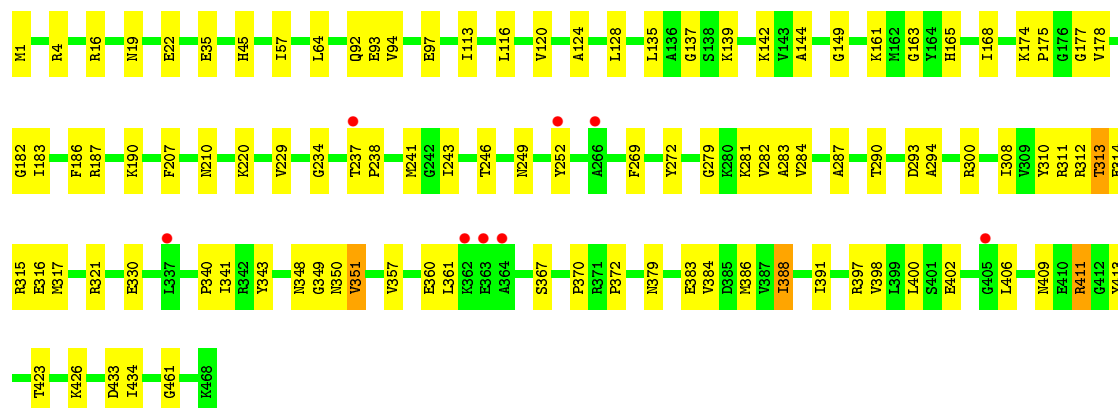
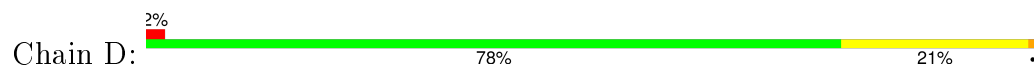
- Molecule 2: Dihydropyrimidine dehydrogenase subunit A







● Molecule 2: Dihydropyrimidine dehydrogenase subunit A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.40 Å 81.40 Å 307.43 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.40 46.07 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.96-2.40) 99.1 (46.07-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	11.30	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.39 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.200 , 0.249 0.201 , 0.250	Depositor DCC
$R_{free}$ test set	3751 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.8	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 28.4	EDS
Estimated twinning fraction	0.457 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 76866 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, SF4, FES, NAD, 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	0.23	0/2178	0.49	0/2939
1	C	0.23	0/2084	0.49	0/2812
2	B	0.23	0/3697	0.46	2/4994 (0.0%)
2	D	0.23	0/3697	0.44	0/4994
All	All	0.23	0/11656	0.47	2/15739 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	133	LYS	C-N-CD	-6.77	105.72	120.60
2	B	133	LYS	C-N-CA	5.05	143.23	122.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2140	0	2188	72	0
1	C	2049	0	2087	58	0
2	B	3625	0	3646	92	1
2	D	3625	0	3646	61	1
3	A	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4	0	0	1	0
4	A	53	0	31	2	0
4	B	53	0	30	5	0
4	C	53	0	31	1	0
4	D	53	0	31	2	0
5	A	44	0	23	5	0
5	D	44	0	24	3	0
6	B	16	0	0	0	0
6	D	16	0	0	0	0
7	D	5	0	0	0	0
8	A	15	0	0	0	0
8	B	56	0	0	1	0
8	C	20	0	0	0	0
8	D	41	0	0	0	0
All	All	11916	0	11737	268	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 11.

All (268) 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)
2:B:341:ILE:HD11	2:B:357:VAL:HG13	1.59	0.82
1:A:178:LEU:HB3	1:A:182:ARG:HG2	1.63	0.79
2:B:19:ASN:O	2:B:300:ARG:NH1	2.17	0.77
1:A:171:VAL:HG22	5:A:503:NAD:H8A	1.66	0.76
1:C:180:ARG:HG2	1:C:181:GLU:H	1.51	0.76
1:C:53:THR:HG21	1:C:117:THR:HG23	1.68	0.75
2:D:290:THR:HA	4:D:503:FAD:HM73	1.69	0.75
1:A:16:ALA:HB3	1:A:19:VAL:HB	1.71	0.73
1:A:14:LYS:NZ	1:A:17:GLU:O	2.22	0.73
1:C:229:ARG:HH22	2:D:252:TYR:HA	1.55	0.72
2:B:281:LYS:HG2	2:B:305:LYS:HB2	1.72	0.72
2:B:423:THR:HG23	2:B:425:VAL:H	1.57	0.70
2:B:290:THR:HA	4:B:503:FAD:HM73	1.73	0.70
1:C:10:VAL:HG12	1:C:11:LYS:HG3	1.73	0.70
1:C:77:GLU:HG3	1:C:273:ARG:HD2	1.76	0.68
2:D:313:THR:OG1	2:D:314:GLU:N	2.27	0.68
2:D:300:ARG:NH2	2:D:330:GLU:OE2	2.28	0.67
1:A:53:THR:HG21	1:A:117:THR:HG23	1.77	0.67
1:C:192:PRO:HG2	1:C:195:MET:HG2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ASP:OD1	1:C:162:ASP:N	2.29	0.66
1:A:18:ASP:N	1:A:18:ASP:OD1	2.29	0.66
2:B:142:LYS:HA	2:B:165:HIS:HB2	1.77	0.66
2:D:35:GLU:HB3	2:D:116:LEU:HD21	1.77	0.65
2:D:290:THR:H	5:D:504:NAD:H4N	1.61	0.65
2:B:300:ARG:NH2	2:B:330:GLU:OE2	2.29	0.65
2:D:183:ILE:O	2:D:190:LYS:NZ	2.29	0.65
1:A:229:ARG:NH1	2:B:246:THR:O	2.30	0.65
1:A:266:GLN:HB2	4:A:502:FAD:H3B	1.80	0.64
1:A:22:PHE:HB2	1:A:66:MET:HG3	1.79	0.64
2:D:294:ALA:HB1	2:D:388:ILE:HD12	1.80	0.63
1:A:212:VAL:HG11	1:A:253:TRP:HH2	1.63	0.63
2:D:311:ARG:HG3	2:D:312:ARG:HG2	1.80	0.62
1:A:13:VAL:HG13	1:A:21:ASP:HB3	1.82	0.62
2:B:236:GLY:HA2	2:B:393:GLN:HB3	1.81	0.61
1:A:31:LYS:HG2	1:A:59:PRO:HB3	1.81	0.61
2:B:35:GLU:OE1	2:B:38:ARG:NH1	2.33	0.61
2:B:3:ASN:OD1	2:B:38:ARG:NH2	2.34	0.61
2:D:426:LYS:H	2:D:426:LYS:HD2	1.65	0.61
1:A:100:ILE:HD13	1:A:124:ALA:HB1	1.83	0.60
1:C:113:VAL:HG13	1:C:192:PRO:HG3	1.83	0.60
1:C:212:VAL:HG11	1:C:253:TRP:HH2	1.65	0.59
2:B:183:ILE:O	2:B:190:LYS:NZ	2.27	0.59
1:C:69:LYS:HB2	1:C:115:ILE:HD11	1.85	0.59
2:D:287:ALA:HB1	2:D:317:MET:HG3	1.85	0.59
2:D:144:ALA:HB3	2:D:229:VAL:HG12	1.85	0.58
2:B:14:GLU:O	2:B:18:ARG:NH1	2.36	0.58
1:C:216:PRO:HG2	1:C:228:CYS:HB2	1.86	0.58
1:A:212:VAL:HG11	1:A:253:TRP:CH2	2.38	0.58
1:A:140:THR:HG22	1:A:141:LYS:H	1.67	0.57
2:B:24:ALA:O	2:B:118:ARG:NH2	2.37	0.57
1:C:18:ASP:N	1:C:18:ASP:OD1	2.35	0.57
1:C:200:THR:HG23	1:C:207:GLY:H	1.70	0.57
2:D:409:ASN:HD21	2:D:413:TYR:HB2	1.68	0.57
1:A:161:ASP:OD1	1:A:162:ASP:N	2.37	0.57
1:C:112:GLY:HA2	1:C:138:ALA:HA	1.86	0.57
1:C:143:TYR:HD1	1:C:144:LEU:HD12	1.70	0.57
1:C:161:ASP:HB2	1:C:165:ALA:HB3	1.87	0.56
2:B:358:ARG:HG2	2:B:378:SER:HB3	1.87	0.56
2:D:400:LEU:HD21	2:D:434:ILE:HD11	1.87	0.56
1:A:117:THR:HB	1:A:190:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:NE	5:A:503:NAD:O1N	2.37	0.56
2:D:178:VAL:HG13	2:D:182:GLY:HA3	1.88	0.56
1:A:262:GLN:HG2	2:B:277:ARG:HD2	1.86	0.56
2:D:93:GLU:HG2	2:D:94:VAL:HG13	1.87	0.56
1:A:107:LEU:HB2	1:A:183:LYS:HD2	1.89	0.55
2:B:16:ARG:HD2	2:B:23:VAL:HG22	1.88	0.55
2:B:143:VAL:HG12	2:B:228:ALA:HB3	1.88	0.55
2:D:313:THR:HG23	2:D:316:GLU:HG3	1.87	0.55
2:B:360:GLU:HB3	2:B:375:ILE:HD11	1.89	0.55
2:B:22:GLU:HA	2:B:186:PHE:HA	1.88	0.55
2:D:348:ASN:O	2:D:350:ASN:N	2.38	0.55
1:C:11:LYS:HB2	1:C:23:TRP:HB2	1.90	0.54
1:C:65:ARG:HH22	1:C:147:VAL:HG21	1.73	0.54
2:B:409:ASN:OD1	2:B:413:TYR:N	2.41	0.53
1:C:180:ARG:HG2	1:C:181:GLU:N	2.20	0.53
2:D:283:ALA:HB2	2:D:384:VAL:HG11	1.89	0.53
1:A:115:ILE:HD13	1:A:136:LEU:HG	1.91	0.53
1:C:102:ASN:OD1	1:C:102:ASN:N	2.41	0.53
1:A:151:LYS:O	1:A:155:ASP:N	2.38	0.53
2:B:16:ARG:O	2:B:300:ARG:NH1	2.42	0.53
2:D:282:VAL:HG22	2:D:386:MET:HB3	1.90	0.53
1:A:205:GLU:HG2	1:A:208:VAL:HG13	1.90	0.52
2:D:310:TYR:CE2	2:D:312:ARG:HB2	2.44	0.52
1:C:16:ALA:HB3	1:C:19:VAL:HB	1.90	0.52
2:D:281:LYS:NZ	2:D:383:GLU:OE1	2.40	0.52
2:B:369:ARG:HB3	2:B:370:PRO:HD3	1.91	0.52
2:B:423:THR:OG1	2:B:424:SER:N	2.42	0.52
2:D:241:MET:SD	2:D:340:PRO:HG2	2.50	0.51
2:B:57:ILE:HG21	2:B:113:ILE:HD13	1.91	0.51
1:A:263:TYR:OH	2:B:252:TYR:OH	2.28	0.51
2:D:135:LEU:O	2:D:163:GLY:HA2	2.09	0.51
2:B:409:ASN:N	2:B:413:TYR:O	2.43	0.51
1:A:109:VAL:HG21	1:A:175:MET:SD	2.50	0.51
1:A:42:ARG:NE	1:A:89:ASP:OD2	2.31	0.51
1:C:73:LYS:HB2	1:C:270:SER:HA	1.93	0.51
1:A:46:LYS:HG2	1:C:103:TYR:HB2	1.93	0.51
1:C:114:GLY:H	1:C:192:PRO:HD3	1.75	0.51
2:B:260:ARG:NH1	2:B:275:PRO:O	2.44	0.51
2:D:284:VAL:HB	2:D:308:ILE:HD13	1.92	0.51
2:B:351:VAL:O	2:B:385:ASP:HA	2.11	0.51
2:D:135:LEU:HD12	2:D:161:LYS:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:THR:O	2:B:466:TRP:NE1	2.42	0.50
2:B:4:ARG:HD3	2:B:109:GLU:HG3	1.93	0.50
2:D:316:GLU:OE1	2:D:370:PRO:HG2	2.10	0.50
1:A:46:LYS:NZ	2:B:271:GLU:OE1	2.35	0.50
1:A:226:GLY:N	3:A:501:FES:S2	2.82	0.50
2:B:14:GLU:HA	2:B:17:ARG:HD2	1.93	0.50
1:A:218:MET:HG2	1:A:228:CYS:HB3	1.93	0.50
2:B:339:LEU:HD12	2:B:340:PRO:HD2	1.94	0.50
2:B:181:TYR:OH	4:B:503:FAD:H3B	2.12	0.50
2:D:234:GLY:HA2	2:D:433:ASP:HB2	1.93	0.50
2:B:308:ILE:HB	2:B:334:PHE:HA	1.94	0.49
1:A:202:LYS:O	1:A:204:ARG:N	2.45	0.49
2:B:89:VAL:O	4:B:503:FAD:N3	2.39	0.49
1:A:34:ARG:HB3	1:A:97:PRO:HB3	1.94	0.49
2:D:45:HIS:ND1	2:D:45:HIS:O	2.44	0.49
2:D:187:ARG:NE	2:D:293:ASP:OD1	2.45	0.49
1:A:175:MET:HE3	1:A:202:LYS:HB2	1.95	0.49
1:A:105:ASN:HB2	1:A:183:LYS:HB2	1.94	0.49
1:A:48:GLU:OE2	1:A:74:THR:OG1	2.31	0.49
1:C:183:LYS:HG2	1:C:184:PHE:H	1.78	0.49
1:C:91:VAL:HG12	2:D:210:ASN:HB3	1.94	0.49
1:C:167:MET:HG3	1:C:168:LYS:H	1.77	0.49
1:A:43:LEU:HD21	1:A:78:LEU:HD13	1.95	0.49
1:A:189:ALA:HB3	1:A:212:VAL:HG22	1.95	0.49
2:D:409:ASN:ND2	2:D:413:TYR:O	2.46	0.49
2:D:57:ILE:HD13	2:D:113:ILE:HD13	1.94	0.49
1:A:159:VAL:O	1:A:166:GLY:HA3	2.13	0.48
2:D:241:MET:HG3	2:D:391:ILE:HD13	1.94	0.48
2:B:134:PRO:HB3	2:B:204:GLY:HA3	1.95	0.48
2:B:133:LYS:HB3	2:B:134:PRO:HA	1.94	0.48
2:D:243:ILE:HD11	2:D:343:TYR:CZ	2.48	0.48
1:C:215:ASN:HA	4:C:502:FAD:HM83	1.95	0.48
1:A:204:ARG:HG3	1:A:205:GLU:H	1.78	0.48
2:D:311:ARG:HH21	5:D:504:NAD:PN	2.36	0.48
2:B:143:VAL:HG21	2:B:159:LEU:HD13	1.94	0.48
2:D:249:ASN:O	2:D:351:VAL:HG22	2.14	0.48
2:B:62:ARG:O	2:B:65:ARG:HG2	2.14	0.47
1:C:238:PHE:HE2	2:D:238:PRO:HD2	1.79	0.47
2:B:10:GLU:HG2	2:B:24:ALA:HA	1.95	0.47
2:B:41:GLN:HE22	2:B:62:ARG:HH11	1.63	0.47
1:A:211:TRP:CE2	1:A:247:ARG:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:168:ILE:HG23	2:D:207:PHE:HA	1.97	0.47
1:C:136:LEU:HD21	1:C:151:LYS:NZ	2.29	0.47
2:D:142:LYS:HG2	2:D:165:HIS:HB2	1.97	0.47
2:D:22:GLU:HA	2:D:186:PHE:HA	1.95	0.47
1:C:136:LEU:HD13	1:C:146:MET:HB2	1.97	0.47
1:A:172:THR:HG21	1:A:198:PHE:HB3	1.97	0.47
1:A:170:VAL:HG13	5:A:503:NAD:C8A	2.45	0.47
1:C:119:TYR:CE1	1:C:150:PHE:HB3	2.50	0.46
1:C:136:LEU:HG	1:C:157:LEU:HD11	1.97	0.46
1:C:152:GLU:HG3	1:C:157:LEU:HD23	1.98	0.46
1:C:225:CYS:SG	1:C:226:GLY:N	2.89	0.46
2:D:92:GLN:HB3	2:D:97:GLU:HG3	1.98	0.46
2:B:124:ALA:HB1	2:B:128:LEU:HD22	1.97	0.46
2:B:86:CYS:O	2:B:90:CYS:HB2	2.16	0.46
2:B:311:ARG:HG2	2:B:339:LEU:HD13	1.98	0.46
2:B:288:GLY:HA2	2:B:318:PRO:HG2	1.97	0.46
2:D:1:MET:HA	2:D:4:ARG:HE	1.80	0.46
2:D:398:VAL:O	2:D:402:GLU:HG3	2.16	0.46
1:A:202:LYS:O	1:A:205:GLU:N	2.49	0.46
1:A:170:VAL:HG12	1:A:172:THR:H	1.81	0.46
2:D:137:GLY:HA2	2:D:165:HIS:CE1	2.51	0.46
2:D:411:ARG:HG2	2:D:413:TYR:HE2	1.81	0.45
1:C:43:LEU:HD23	1:C:87:ILE:HG23	1.98	0.45
2:D:149:GLY:HA2	2:D:177:GLY:HA3	1.99	0.45
2:B:426:LYS:HA	2:B:466:TRP:CD2	2.51	0.45
1:A:266:GLN:HE21	2:B:275:PRO:HG3	1.82	0.45
2:B:34:GLU:O	2:B:37:GLN:HG2	2.16	0.45
2:B:177:GLY:HA2	4:B:503:FAD:H3B	1.99	0.45
2:B:423:THR:HG22	2:B:428:VAL:O	2.16	0.45
1:C:269:ILE:HG23	1:C:272:GLU:HG2	1.98	0.45
2:B:283:ALA:HB2	2:B:384:VAL:HG11	1.99	0.45
2:D:64:LEU:HD13	2:D:120:VAL:HG22	1.99	0.45
1:A:195:MET:HG3	5:A:503:NAD:C8A	2.47	0.44
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.84	0.44
1:A:212:VAL:O	1:A:245:GLU:HA	2.17	0.44
2:D:360:GLU:O	2:D:372:PRO:HA	2.17	0.44
1:A:258:LYS:HD2	2:B:349:GLY:HA3	1.99	0.44
1:A:75:THR:HG23	4:A:502:FAD:O1P	2.17	0.44
2:B:451:ALA:O	2:B:455:ILE:HG13	2.16	0.44
1:A:229:ARG:HH11	2:B:246:THR:HG22	1.82	0.44
1:C:125:LEU:O	1:C:130:ASN:ND2	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ASN:O	2:B:351:VAL:HG23	2.18	0.44
1:C:68:VAL:HG11	1:C:78:LEU:HD23	2.00	0.44
1:A:205:GLU:HB3	1:A:206:PHE:H	1.49	0.44
1:C:262:GLN:HG3	1:C:263:TYR:CD1	2.53	0.44
2:B:396:ASN:ND2	8:B:613:HOH:O	2.51	0.44
2:B:245:GLY:HA3	2:B:343:TYR:HB2	1.99	0.44
2:D:16:ARG:O	2:D:300:ARG:NH1	2.51	0.44
1:C:218:MET:HG2	1:C:228:CYS:HB3	2.00	0.43
1:A:43:LEU:HD23	1:A:87:ILE:HG23	2.00	0.43
2:B:45:HIS:ND1	2:B:45:HIS:O	2.51	0.43
2:B:408:LEU:HD12	2:B:409:ASN:O	2.18	0.43
2:B:175:PRO:HA	2:B:176:GLY:HA2	1.80	0.43
2:B:1:MET:N	2:B:4:ARG:HH21	2.15	0.43
1:C:136:LEU:HD21	1:C:151:LYS:HZ3	1.83	0.43
1:C:46:LYS:HA	2:D:272:TYR:CD2	2.53	0.43
2:D:341:ILE:HD11	2:D:357:VAL:HG22	2.01	0.43
1:A:265:GLU:HB3	1:A:268:LYS:HE3	2.01	0.43
1:A:272:GLU:O	1:A:276:LYS:NZ	2.47	0.43
1:C:114:GLY:N	1:C:192:PRO:HD3	2.33	0.43
2:B:38:ARG:NH1	2:B:111:VAL:HA	2.34	0.43
2:B:146:VAL:HG13	2:B:213:VAL:HG21	2.01	0.43
2:B:63:LYS:HA	2:B:63:LYS:HD3	1.68	0.43
2:B:316:GLU:OE2	2:B:370:PRO:HG2	2.19	0.42
2:B:9:LYS:HB3	2:B:25:LEU:HD12	2.01	0.42
2:B:74:ARG:HA	2:B:74:ARG:HD3	1.77	0.42
1:A:182:ARG:NH1	1:A:205:GLU:O	2.53	0.42
2:B:131:ASP:OD2	2:B:133:LYS:HG2	2.19	0.42
2:D:243:ILE:O	2:D:246:THR:OG1	2.29	0.42
2:D:139:LYS:HD2	2:D:139:LYS:HA	1.85	0.42
2:B:310:TYR:OH	2:B:312:ARG:HD2	2.19	0.42
2:B:41:GLN:NE2	2:B:62:ARG:HD3	2.34	0.42
2:D:174:LYS:HA	2:D:175:PRO:HD3	1.78	0.42
1:C:13:VAL:O	1:C:21:ASP:HB3	2.19	0.42
2:B:100:CYS:SG	2:B:102:VAL:HG22	2.59	0.42
2:B:399:LEU:HD22	4:B:503:FAD:H61A	1.83	0.42
1:A:123:LYS:O	1:A:127:GLU:N	2.52	0.42
2:B:136:ALA:HA	2:B:163:GLY:HA2	2.00	0.42
1:A:147:VAL:HG12	1:A:149:GLU:HG3	2.02	0.42
2:D:290:THR:H	5:D:504:NAD:C4N	2.32	0.42
1:C:102:ASN:HD22	1:C:186:ILE:HG12	1.84	0.42
1:C:106:VAL:HG21	1:C:125:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ILE:HG13	1:C:262:GLN:HE21	1.84	0.42
1:C:96:ASN:ND2	1:C:241:VAL:O	2.53	0.42
2:B:367:SER:N	2:B:371:ARG:HD2	2.34	0.42
2:D:19:ASN:O	2:D:300:ARG:NH1	2.42	0.42
2:B:9:LYS:HB2	2:B:9:LYS:HE3	1.84	0.42
2:B:464:ASN:HA	2:B:465:PRO:HD2	1.93	0.42
1:C:100:ILE:HG21	1:C:124:ALA:HB1	2.01	0.42
2:B:148:SER:O	2:B:176:GLY:HA3	2.20	0.42
1:C:72:GLY:O	1:C:76:HIS:N	2.46	0.42
1:A:160:THR:HG21	1:A:171:VAL:HA	2.02	0.41
2:B:299:LEU:HA	2:B:303:ALA:HB3	2.02	0.41
1:A:171:VAL:HG13	5:A:503:NAD:O2B	2.20	0.41
1:C:226:GLY:N	3:C:501:FES:S2	2.86	0.41
1:C:267:GLU:N	1:C:267:GLU:OE1	2.52	0.41
2:B:241:MET:HG3	2:B:391:ILE:HD13	2.01	0.41
2:B:339:LEU:HA	2:B:340:PRO:HD2	1.81	0.41
4:D:503:FAD:H9	4:D:503:FAD:H1'1	1.87	0.41
1:A:266:GLN:O	1:A:269:ILE:HG12	2.20	0.41
1:A:22:PHE:CZ	1:A:78:LEU:HG	2.56	0.41
2:B:251:VAL:HG23	2:B:351:VAL:HG21	2.02	0.41
1:C:105:ASN:HB2	1:C:184:PHE:O	2.20	0.41
2:B:133:LYS:HA	2:B:133:LYS:HD3	1.81	0.41
1:C:265:GLU:O	1:C:269:ILE:HG12	2.20	0.41
1:A:103:TYR:CB	1:A:186:ILE:HD11	2.51	0.41
2:B:16:ARG:HA	2:B:19:ASN:OD1	2.20	0.41
1:A:18:ASP:OD1	1:A:144:LEU:HD21	2.20	0.41
2:D:311:ARG:HH22	2:D:312:ARG:HH21	1.69	0.41
1:A:46:LYS:CG	1:C:103:TYR:HB2	2.51	0.41
2:D:124:ALA:O	2:D:128:LEU:HB3	2.21	0.41
2:B:145:VAL:HB	2:B:168:ILE:HG12	2.03	0.41
1:C:161:ASP:OD2	1:C:164:SER:HB2	2.21	0.41
2:B:124:ALA:HA	2:B:128:LEU:HB3	2.03	0.41
1:A:225:CYS:HB2	2:B:256:GLU:HB2	2.03	0.41
1:A:202:LYS:HG2	1:A:205:GLU:HG3	2.03	0.40
1:C:269:ILE:HG13	2:D:269:PHE:CZ	2.56	0.40
2:D:411:ARG:HB3	2:D:413:TYR:CD2	2.57	0.40
1:A:58:LYS:O	1:A:62:GLY:N	2.54	0.40
1:A:175:MET:HB2	1:A:175:MET:HE2	1.71	0.40
2:B:1:MET:HG3	2:B:106:LYS:HE3	2.02	0.40
1:A:77:GLU:HB2	1:A:273:ARG:HH12	1.87	0.40
2:B:324:TYR:CZ	2:B:328:LEU:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:TYR:CE2	2:B:277:ARG:HG3	2.55	0.40
2:B:169:PHE:HA	2:B:208:HIS:HB2	2.03	0.40
1:A:134:THR:O	1:A:157:LEU:HD12	2.21	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)
2:B:365:ASP:OD2	2:D:367:SER:OG[3_554]	2.18	0.02

## 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	274/276 (99%)	251 (92%)	20 (7%)	3 (1%)	17	25
1	C	259/276 (94%)	239 (92%)	18 (7%)	2 (1%)	24	35
2	B	466/468 (100%)	435 (93%)	28 (6%)	3 (1%)	30	43
2	D	466/468 (100%)	441 (95%)	22 (5%)	3 (1%)	30	43
All	All	1465/1488 (98%)	1366 (93%)	88 (6%)	11 (1%)	24	35

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLY
1	A	203	ALA
2	B	364	ALA
1	A	179	PHE
1	C	184	PHE
2	D	349	GLY
2	B	133	LYS

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Mol	Chain	Res	Type
2	D	279	GLY
2	D	461	GLY
2	B	350	ASN
1	C	167	MET

### 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	233/233 (100%)	218 (94%)	15 (6%)	22	34
1	C	224/233 (96%)	215 (96%)	9 (4%)	38	58
2	B	381/381 (100%)	372 (98%)	9 (2%)	57	76
2	D	381/381 (100%)	368 (97%)	13 (3%)	44	65
All	All	1219/1228 (99%)	1173 (96%)	46 (4%)	40	60

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	34	ARG
1	A	113	VAL
1	A	141	LYS
1	A	145	ILE
1	A	149	GLU
1	A	162	ASP
1	A	186	ILE
1	A	206	PHE
1	A	208	VAL
1	A	210	ILE
1	A	231	THR
1	A	247	ARG
1	A	257	LEU
1	A	264	ARG
2	B	8	MET
2	B	81	ASN

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Mol	Chain	Res	Type
2	B	179	LEU
2	B	198	SER
2	B	237	THR
2	B	301	LEU
2	B	321	ARG
2	B	362	LYS
2	B	369	ARG
1	C	13	VAL
1	C	102	ASN
1	C	106	VAL
1	C	156	VAL
1	C	210	ILE
1	C	241	VAL
1	C	257	LEU
1	C	266	GLN
1	C	272	GLU
2	D	220	LYS
2	D	237	THR
2	D	313	THR
2	D	315	ARG
2	D	321	ARG
2	D	351	VAL
2	D	361	LEU
2	D	379	ASN
2	D	388	ILE
2	D	397	ARG
2	D	406	LEU
2	D	411	ARG
2	D	423	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	41	GLN

### 5.3.3 RNA ⓘ

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](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	FES	A	501	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	A	502	-	52,58,58	3.88	19 (36%)	52,89,89	2.50	9 (17%)
5	NAD	A	503	-	42,48,48	4.40	15 (35%)	46,73,73	3.48	13 (28%)
6	SF4	B	501	2	0,12,12	0.00	-	0,24,24	0.00	-
6	SF4	B	502	2	0,12,12	0.00	-	0,24,24	0.00	-
4	FAD	B	503	-	52,58,58	3.89	20 (38%)	52,89,89	2.51	9 (17%)
3	FES	C	501	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	C	502	-	52,58,58	3.84	18 (34%)	52,89,89	2.55	10 (19%)
6	SF4	D	501	2	0,12,12	0.00	-	0,24,24	0.00	-
6	SF4	D	502	2	0,12,12	0.00	-	0,24,24	0.00	-
4	FAD	D	503	-	52,58,58	3.87	18 (34%)	52,89,89	2.60	11 (21%)
5	NAD	D	504	-	42,48,48	4.46	15 (35%)	46,73,73	3.24	13 (28%)
7	PO4	D	505	-	4,4,4	0.68	0	6,6,6	0.23	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	FES	A	501	1	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	A	502	-	-	0/30/50/50	0/6/6/6
5	NAD	A	503	-	-	0/22/62/62	0/5/5/5
6	SF4	B	501	2	-	0/0/48/48	0/6/5/5
6	SF4	B	502	2	-	0/0/48/48	0/6/5/5
4	FAD	B	503	-	-	0/30/50/50	0/6/6/6
3	FES	C	501	1	-	0/0/4/4	0/1/1/1
4	FAD	C	502	-	-	0/30/50/50	0/6/6/6
6	SF4	D	501	2	-	0/0/48/48	0/6/5/5
6	SF4	D	502	2	-	0/0/48/48	0/6/5/5
4	FAD	D	503	-	-	0/30/50/50	0/6/6/6
5	NAD	D	504	-	-	0/22/62/62	0/5/5/5
7	PO4	D	505	-	-	0/0/0/0	0/0/0/0

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	NAD	C2B-C1B	-17.81	1.25	1.53
5	D	504	NAD	C2B-C1B	-17.79	1.25	1.53
4	B	503	FAD	C2B-C1B	-14.48	1.30	1.53
4	D	503	FAD	C2B-C1B	-14.43	1.30	1.53
4	A	502	FAD	C2B-C1B	-14.33	1.30	1.53
4	C	502	FAD	C2B-C1B	-13.90	1.31	1.53
5	A	503	NAD	C3B-C4B	-9.38	1.27	1.53
5	D	504	NAD	C3B-C4B	-9.34	1.28	1.53
5	A	503	NAD	O3B-C3B	-8.14	1.23	1.43
5	D	504	NAD	O3B-C3B	-8.08	1.23	1.43
4	C	502	FAD	O4B-C4B	-6.45	1.30	1.45
4	A	502	FAD	O4B-C4B	-6.41	1.30	1.45
4	B	503	FAD	O4B-C4B	-6.40	1.30	1.45
4	D	503	FAD	O4B-C4B	-6.37	1.30	1.45
5	D	504	NAD	C3D-C4D	-4.98	1.39	1.53
5	A	503	NAD	C3D-C4D	-4.38	1.41	1.53
5	D	504	NAD	C2N-N1N	-2.86	1.30	1.35
5	A	503	NAD	C2N-N1N	-2.75	1.31	1.35
4	B	503	FAD	O3B-C3B	-2.66	1.36	1.43
4	B	503	FAD	O4-C4	-2.64	1.17	1.24
4	C	502	FAD	O4-C4	-2.63	1.17	1.24
4	D	503	FAD	O3B-C3B	-2.58	1.36	1.43
4	C	502	FAD	O3B-C3B	-2.57	1.36	1.43
4	D	503	FAD	O4-C4	-2.56	1.18	1.24
4	A	502	FAD	O4-C4	-2.55	1.18	1.24
4	A	502	FAD	O3B-C3B	-2.54	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	504	NAD	O2D-C2D	-2.43	1.37	1.43
5	A	503	NAD	C2D-C1D	-2.37	1.49	1.53
5	A	503	NAD	O2D-C2D	-2.27	1.37	1.43
5	D	504	NAD	C2D-C1D	-2.14	1.50	1.53
4	B	503	FAD	C4'-C3'	-2.07	1.49	1.53
4	B	503	FAD	C5A-C4A	-2.01	1.36	1.40
4	A	502	FAD	C5A-C4A	-2.01	1.36	1.40
5	A	503	NAD	C5B-C4B	2.01	1.58	1.51
5	D	504	NAD	C5B-C4B	2.14	1.58	1.51
4	D	503	FAD	C2A-N1A	2.39	1.38	1.33
4	A	502	FAD	C2A-N1A	2.39	1.38	1.33
4	C	502	FAD	C2A-N1A	2.42	1.38	1.33
4	B	503	FAD	C2A-N1A	2.44	1.38	1.33
5	A	503	NAD	C6A-N6A	2.62	1.44	1.34
5	D	504	NAD	C3N-C7N	2.68	1.54	1.50
5	D	504	NAD	C6A-N6A	2.71	1.45	1.34
4	B	503	FAD	C10-N10	2.74	1.42	1.39
5	A	503	NAD	C3N-C7N	2.83	1.55	1.50
4	D	503	FAD	C10-N10	2.90	1.42	1.39
4	A	502	FAD	C10-N10	2.93	1.42	1.39
4	C	502	FAD	C10-N10	2.95	1.42	1.39
5	A	503	NAD	O4B-C4B	2.99	1.51	1.45
4	C	502	FAD	C6A-N6A	3.02	1.46	1.34
4	B	503	FAD	C6A-N6A	3.02	1.46	1.34
4	D	503	FAD	C6A-N6A	3.03	1.46	1.34
4	D	503	FAD	C2A-N3A	3.05	1.37	1.32
4	A	502	FAD	C6A-N6A	3.06	1.46	1.34
4	C	502	FAD	C2A-N3A	3.06	1.37	1.32
5	D	504	NAD	O4B-C4B	3.08	1.52	1.45
4	A	502	FAD	C2A-N3A	3.10	1.37	1.32
4	B	503	FAD	C2A-N3A	3.13	1.37	1.32
4	B	503	FAD	O2B-C2B	3.39	1.50	1.43
4	A	502	FAD	O2B-C2B	3.41	1.51	1.43
4	C	502	FAD	O2B-C2B	3.42	1.51	1.43
4	D	503	FAD	O2B-C2B	3.45	1.51	1.43
4	C	502	FAD	C4-C4X	3.52	1.48	1.41
4	B	503	FAD	C4-C4X	3.55	1.48	1.41
4	D	503	FAD	C4-C4X	3.71	1.48	1.41
4	A	502	FAD	C4-C4X	3.75	1.48	1.41
5	A	503	NAD	O4D-C1D	3.78	1.46	1.41
4	A	502	FAD	C2-N1	3.93	1.46	1.38
4	D	503	FAD	C2-N1	3.94	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	FAD	C2-N3	4.03	1.46	1.38
4	D	503	FAD	C2-N3	4.04	1.46	1.38
4	C	502	FAD	C2-N3	4.05	1.46	1.38
4	A	502	FAD	C2-N3	4.08	1.46	1.38
4	B	503	FAD	C2-N1	4.11	1.46	1.38
4	C	502	FAD	C2-N1	4.12	1.46	1.38
4	C	502	FAD	C10-N1	4.19	1.42	1.35
4	D	503	FAD	C10-N1	4.20	1.42	1.35
4	A	502	FAD	C10-N1	4.27	1.42	1.35
4	B	503	FAD	C10-N1	4.30	1.43	1.35
5	D	504	NAD	O4D-C1D	4.39	1.47	1.41
5	A	503	NAD	C2B-C3B	4.97	1.66	1.53
5	D	504	NAD	C2B-C3B	5.21	1.67	1.53
5	D	504	NAD	C7N-N7N	5.29	1.43	1.33
4	B	503	FAD	C4-N3	5.31	1.42	1.33
5	A	503	NAD	C7N-N7N	5.34	1.43	1.33
4	C	502	FAD	C4-N3	5.36	1.42	1.33
4	A	502	FAD	C4-N3	5.36	1.42	1.33
4	D	503	FAD	C4-N3	5.39	1.42	1.33
4	C	502	FAD	C5X-N5	6.71	1.45	1.35
4	D	503	FAD	C9A-N10	6.80	1.48	1.38
4	A	502	FAD	C5X-N5	6.93	1.46	1.35
4	D	503	FAD	C5X-N5	6.93	1.46	1.35
4	B	503	FAD	C5X-N5	6.93	1.46	1.35
4	B	503	FAD	C4X-N5	6.95	1.44	1.33
4	C	502	FAD	C4X-N5	6.96	1.44	1.33
4	B	503	FAD	C9A-N10	7.03	1.48	1.38
4	C	502	FAD	C9A-N10	7.07	1.48	1.38
4	D	503	FAD	C4X-N5	7.08	1.44	1.33
4	A	502	FAD	C9A-N10	7.08	1.48	1.38
4	A	502	FAD	C4X-N5	7.20	1.44	1.33
5	A	503	NAD	O4B-C1B	13.64	1.60	1.41
5	D	504	NAD	O4B-C1B	14.02	1.61	1.41
4	D	503	FAD	O4B-C1B	14.50	1.61	1.41
4	A	502	FAD	O4B-C1B	14.52	1.62	1.41
4	B	503	FAD	O4B-C1B	14.61	1.62	1.41
4	C	502	FAD	O4B-C1B	14.66	1.62	1.41

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	FAD	N3A-C2A-N1A	-11.30	120.00	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	FAD	N3A-C2A-N1A	-11.21	120.07	128.87
4	C	502	FAD	N3A-C2A-N1A	-11.20	120.08	128.87
4	A	502	FAD	N3A-C2A-N1A	-11.17	120.10	128.87
5	A	503	NAD	N3A-C2A-N1A	-9.47	121.43	128.87
5	D	504	NAD	N3A-C2A-N1A	-9.42	121.47	128.87
5	A	503	NAD	C4B-O4B-C1B	-7.81	101.37	109.64
5	D	504	NAD	C4B-O4B-C1B	-6.88	102.35	109.64
5	A	503	NAD	O3B-C3B-C4B	-6.56	91.41	111.01
5	D	504	NAD	O3B-C3B-C4B	-6.42	91.84	111.01
4	D	503	FAD	N6A-C6A-N1A	-5.80	108.78	118.52
4	A	502	FAD	N6A-C6A-N1A	-5.62	109.08	118.52
4	C	502	FAD	N6A-C6A-N1A	-5.57	109.17	118.52
4	B	503	FAD	N6A-C6A-N1A	-5.55	109.20	118.52
4	D	503	FAD	C7M-C7-C6	-5.38	105.12	120.33
4	A	502	FAD	C7M-C7-C6	-5.25	105.50	120.33
4	C	502	FAD	C7M-C7-C6	-5.17	105.71	120.33
4	B	503	FAD	C7M-C7-C6	-5.07	106.00	120.33
4	B	503	FAD	N3-C2-N1	-4.76	119.68	127.69
4	D	503	FAD	N3-C2-N1	-4.70	119.78	127.69
4	A	502	FAD	N3-C2-N1	-4.68	119.81	127.69
4	C	502	FAD	C4B-O4B-C1B	-4.65	104.71	109.64
4	C	502	FAD	N3-C2-N1	-4.58	119.97	127.69
4	D	503	FAD	C4B-O4B-C1B	-4.27	105.11	109.64
5	A	503	NAD	O4D-C4D-C3D	-3.05	98.98	105.16
4	D	503	FAD	C4X-C4-N3	-3.00	119.60	123.52
5	D	504	NAD	O2D-C2D-C3D	-2.99	102.18	111.86
4	A	502	FAD	C4X-C4-N3	-2.94	119.67	123.52
5	D	504	NAD	O4D-C4D-C3D	-2.91	99.26	105.16
5	A	503	NAD	C5N-C4N-C3N	-2.91	116.88	120.35
5	D	504	NAD	C5N-C4N-C3N	-2.82	116.98	120.35
4	B	503	FAD	C4X-C4-N3	-2.79	119.88	123.52
4	C	502	FAD	C4X-C4-N3	-2.77	119.90	123.52
5	A	503	NAD	C2B-C1B-N9A	-2.58	106.55	113.47
5	A	503	NAD	O2D-C2D-C3D	-2.36	104.22	111.86
4	D	503	FAD	C1B-N9A-C4A	-2.01	124.56	126.81
5	D	504	NAD	O2A-PA-O3	2.27	115.01	105.27
5	D	504	NAD	O4D-C4D-C5D	2.40	117.86	109.29
5	A	503	NAD	O4D-C4D-C5D	2.40	117.89	109.29
5	D	504	NAD	N6A-C6A-N1A	2.48	122.68	118.52
5	A	503	NAD	O2A-PA-O3	2.48	115.91	105.27
4	C	502	FAD	C4X-N5-C5X	2.76	119.97	116.72
4	D	503	FAD	C4X-N5-C5X	2.93	120.17	116.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	FAD	C4X-N5-C5X	2.96	120.22	116.72
5	A	503	NAD	N6A-C6A-N1A	3.04	123.62	118.52
4	B	503	FAD	C4X-N5-C5X	3.05	120.31	116.72
5	D	504	NAD	C2D-C1D-N1N	3.23	119.86	113.53
4	A	502	FAD	C5X-C9A-N10	3.25	120.01	117.58
5	D	504	NAD	C4D-O4D-C1D	3.33	113.18	109.64
4	D	503	FAD	C5X-C9A-N10	3.45	120.16	117.58
4	C	502	FAD	C5X-C9A-N10	3.51	120.21	117.58
4	B	503	FAD	C5X-C9A-N10	3.57	120.25	117.58
5	A	503	NAD	C2D-C1D-N1N	3.74	120.86	113.53
5	D	504	NAD	C2D-C3D-C4D	3.84	110.50	102.64
5	A	503	NAD	C2D-C3D-C4D	5.03	112.94	102.64
4	C	502	FAD	C4-N3-C2	5.11	119.42	115.16
4	A	502	FAD	C4-N3-C2	5.59	119.82	115.16
4	D	503	FAD	C4-N3-C2	5.65	119.87	115.16
4	B	503	FAD	C4-N3-C2	5.68	119.89	115.16
4	B	503	FAD	C7M-C7-C8	6.05	133.74	120.73
4	D	503	FAD	C7M-C7-C8	6.32	134.33	120.73
4	A	502	FAD	C7M-C7-C8	6.34	134.38	120.73
4	C	502	FAD	C7M-C7-C8	6.38	134.45	120.73
5	D	504	NAD	O4D-C1D-N1N	14.13	123.36	108.10
5	A	503	NAD	O4D-C1D-N1N	15.63	124.98	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	FES	1	0
4	A	502	FAD	2	0
5	A	503	NAD	5	0
4	B	503	FAD	5	0
3	C	501	FES	1	0
4	C	502	FAD	1	0
4	D	503	FAD	2	0
5	D	504	NAD	3	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	276/276 (100%)	-0.22	2 (0%) 89 88	35, 52, 89, 118	0
1	C	265/276 (96%)	0.31	23 (8%) 13 12	45, 66, 127, 201	0
2	B	468/468 (100%)	-0.30	9 (1%) 70 69	26, 43, 92, 181	0
2	D	468/468 (100%)	-0.34	8 (1%) 73 72	28, 43, 81, 165	0
All	All	1477/1488 (99%)	-0.19	42 (2%) 56 55	26, 49, 99, 201	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	115	ILE	10.2
1	C	100	ILE	9.0
1	C	271	TYR	6.6
1	C	112	GLY	6.5
2	D	363	GLU	6.2
1	C	15	ILE	6.0
1	C	114	GLY	5.8
1	C	190	VAL	5.7
2	B	391	ILE	5.5
2	B	370	PRO	5.2
1	C	116	ALA	4.5
2	D	237	THR	4.1
1	C	188	TRP	4.1
1	A	206	PHE	3.6
1	C	274	PHE	3.6
2	D	364	ALA	3.5
2	B	132	VAL	3.5
1	C	160	THR	3.4
1	C	109	VAL	3.2
2	D	266	ALA	3.1
2	D	362	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	206	PHE	3.0
1	C	143	TYR	3.0
2	B	363	GLU	2.9
2	B	362	LYS	2.8
2	B	347	ALA	2.8
1	C	91	VAL	2.7
1	C	246	PHE	2.7
2	B	468	LYS	2.5
1	C	170	VAL	2.5
1	A	184	PHE	2.5
2	B	125	ALA	2.4
2	D	337	LEU	2.4
1	C	172	THR	2.4
1	C	208	VAL	2.2
1	C	257	LEU	2.2
1	C	99	GLU	2.1
1	C	4	THR	2.1
1	C	186	ILE	2.1
2	D	252	TYR	2.1
2	B	367	SER	2.1
2	D	405	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	SF4	D	502	8/8	0.95	0.22	6.20	35,43,62,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SF4	B	502	8/8	0.96	0.20	3.38	33,37,57,81	0
6	SF4	D	501	8/8	0.98	0.19	2.85	29,36,53,59	0
6	SF4	B	501	8/8	0.98	0.18	2.75	27,43,49,50	0
5	NAD	D	504	44/44	0.94	0.14	0.48	14,73,110,114	0
3	FES	A	501	4/4	0.96	0.14	0.36	30,45,62,69	0
4	FAD	A	502	53/53	0.96	0.14	0.10	23,48,69,79	0
4	FAD	D	503	53/53	0.98	0.13	0.09	13,36,45,47	0
4	FAD	B	503	53/53	0.98	0.13	-0.12	11,28,39,115	0
4	FAD	C	502	53/53	0.96	0.13	-0.34	19,39,54,59	0
5	NAD	A	503	44/44	0.96	0.13	-0.69	20,48,61,91	0
3	FES	C	501	4/4	0.98	0.11	-0.91	35,36,39,40	0
7	PO4	D	505	5/5	0.97	0.11	-	48,49,55,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.