Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 06:59 PM GMT

PDB ID	:	1H7W
Title	:	DIHYDROPYRIMIDINE DEHYDROGENASE (DPD) FROM PIG
Authors	:	Dobritzsch, D.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on	:	2001-01-19
Resolution	:	1.90 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:

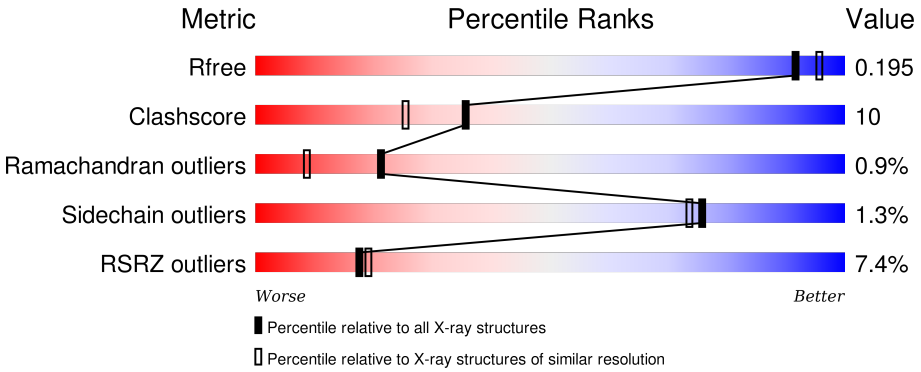
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	1025	7% 81% 17%
1	B	1025	8% 82% 16%
1	C	1025	7% 81% 18%
1	D	1025	8% 82% 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36125 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.

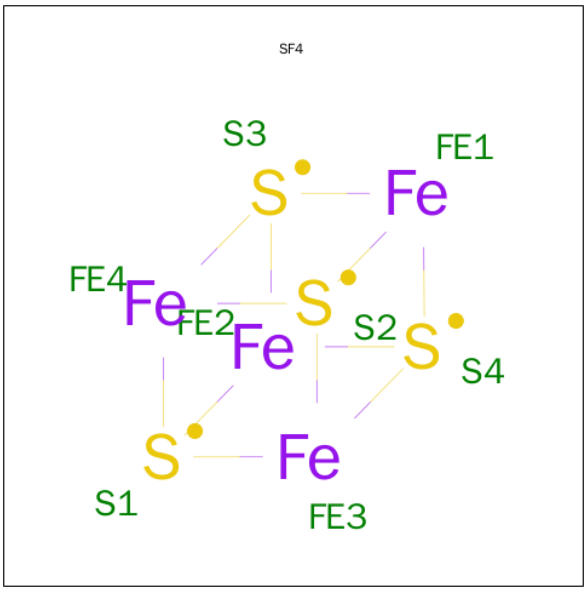
- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1016	Total	C	N	O	S	66	0	0
			7750	4913	1314	1467	56			
1	B	1017	Total	C	N	O	S	70	0	0
			7757	4918	1315	1468	56			
1	C	1016	Total	C	N	O	S	28	0	0
			7750	4913	1314	1467	56			
1	D	1018	Total	C	N	O	S	43	0	0
			7765	4924	1316	1469	56			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	CONFLICT	UNP Q28943
B	60	ASP	GLY	CONFLICT	UNP Q28943
C	60	ASP	GLY	CONFLICT	UNP Q28943
D	60	ASP	GLY	CONFLICT	UNP Q28943

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

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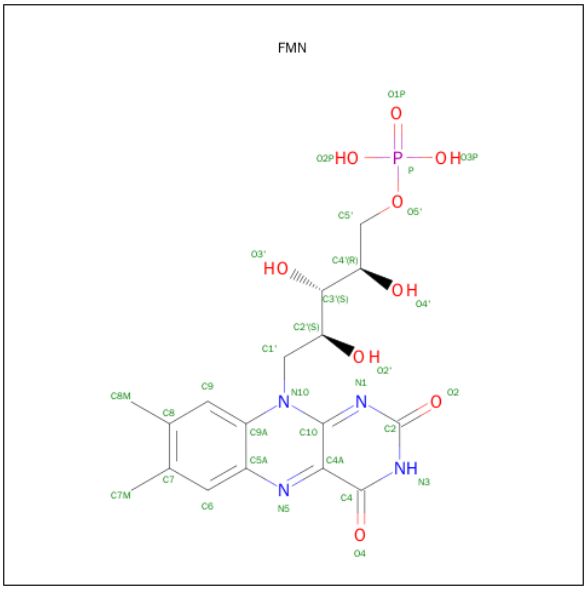
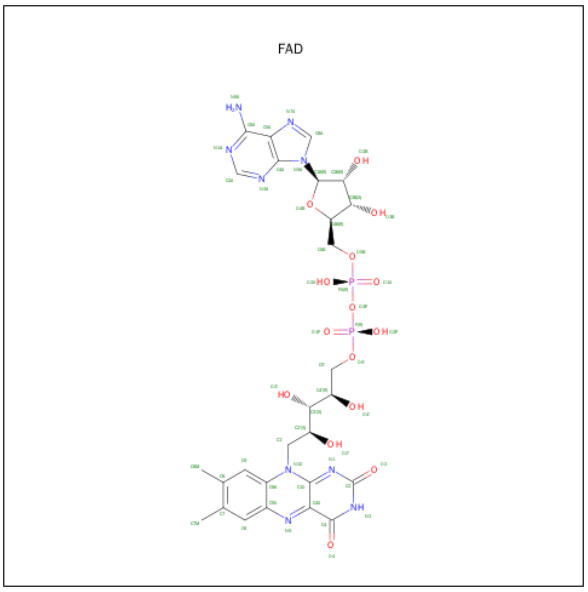
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 17 4 9 1	0	0
3	B	1	Total C N O P 31 17 4 9 1	0	0
3	C	1	Total C N O P 31 17 4 9 1	0	0
3	D	1	Total C N O P 31 17 4 9 1	0	0

- 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 water.

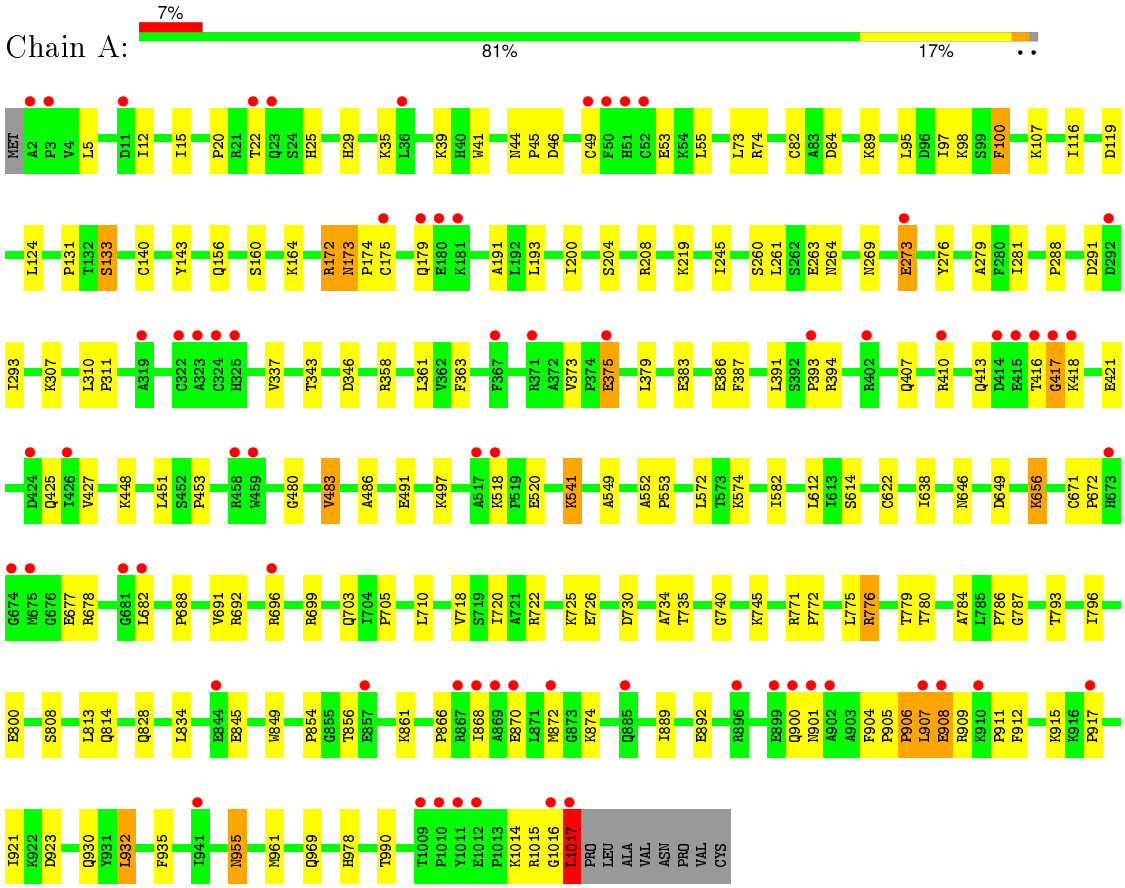
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1148	Total	O	0	0
			1148	1148		
5	B	1125	Total	O	0	0
			1125	1125		
5	C	1176	Total	O	0	0
			1176	1176		
5	D	1190	Total	O	0	0
			1190	1190		

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.

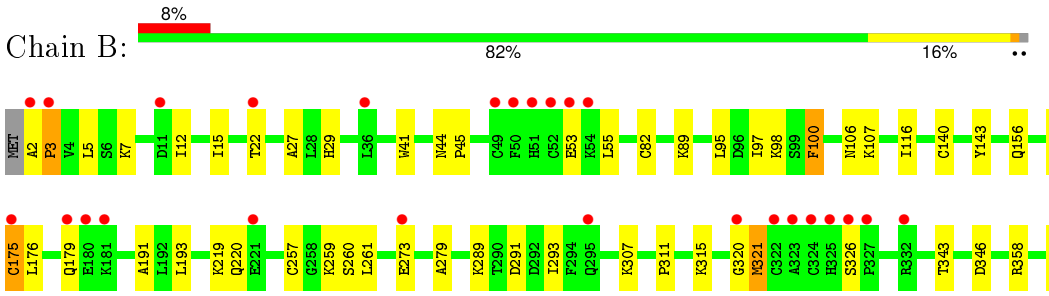
- Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

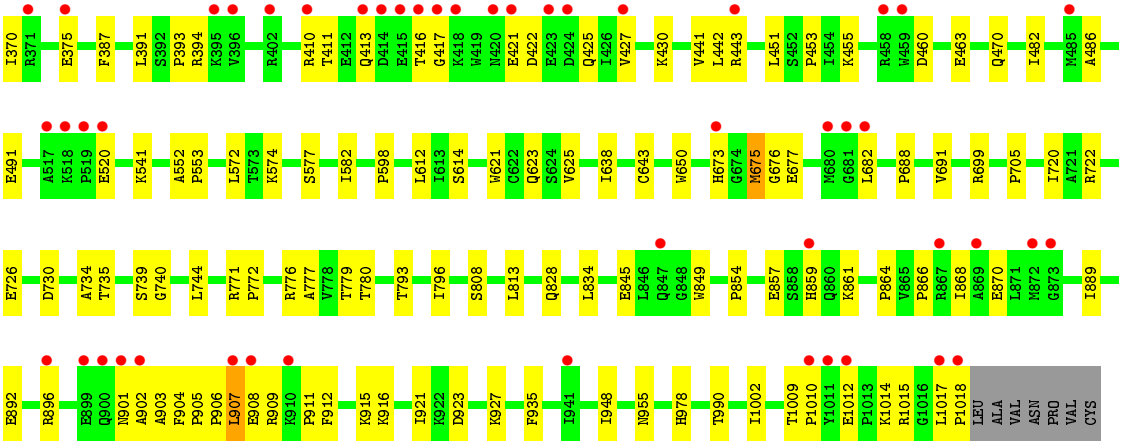
Chain A:



- Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

Chain B:



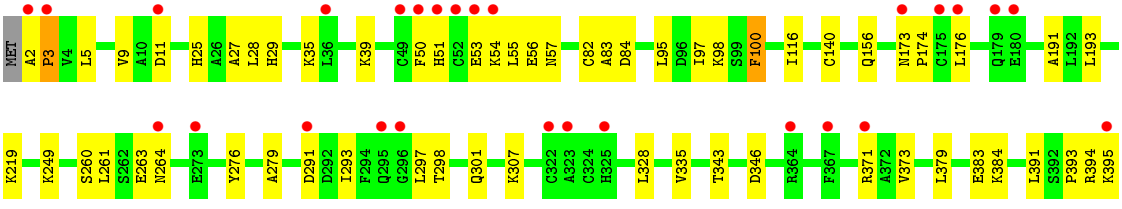


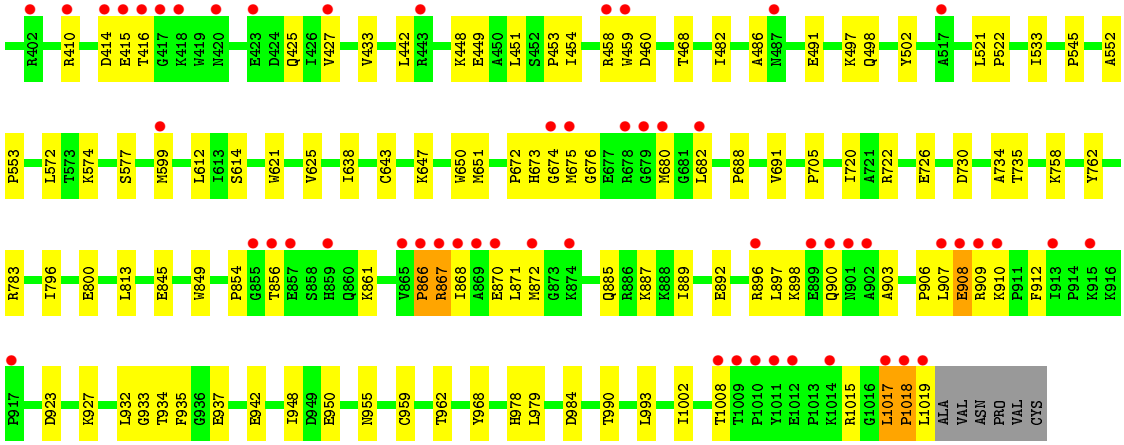
• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

Chain C:

• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

Chain D:




R402 R410 D414 E415 T416 G417 K418 W419 N420 E423 D424 Q425 I426 V427 V433 L442 R443 K448 E449 A450 L451 S452 P453 I454 R458 W459 D460 T468 I482 A486 N487 E491 K497 Q498 Y502 A517 L521 P522 I533 P545 A552
P553 L572 T573 K574 S577 M599 L612 I613 S614 W621 V625 I638 C643 K647 W650 M651 P672 H673 G674 M675 G676 E677 R678 G679 M680 G681 L682 P688 V691 P705 I720 A721 R722 E726 D730 A734 T735 K758 Y762
R783 I796 E800 L813 E845 W849 P854 G855 T856 E857 S858 H859 Q860 K861 V865 P866 R867 I868 A869 E870 L871 M872 G873 K874 Q885 R886 K887 K888 I889 E892 R896 L897 K898 E899 Q900 N901 A902 A903 P906 L907 E908 R909 K910 P911 F912 I913 P914 K915 K916
P917 D923 K927 L932 G933 T934 F935 G936 E937 E942 I948 D949 E950 N955 G959 T962 Y968 H978 L979 D984 T990 L993 I1002 T1008 T1009 P1010 Y1011 E1012 P1013 K1014 R1015 G1016 L1017 P1018 L1019 ALA VAL ASN PRO VAL CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.95Å 159.29Å 163.57Å 90.00° 96.04° 90.00°	Depositor
Resolution (Å)	19.97 – 1.90 24.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.97-1.90) 99.0 (24.99-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	6.83 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.174 , 0.196 0.173 , 0.195	Depositor DCC
R_{free} test set	6483 reflections (2.04%)	DCC
Wilson B-factor (Å^2)	12.7	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 58.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 326044 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	36125	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: FMN, SF4, 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	0.35	0/7911	0.63	4/10721 (0.0%)
1	B	0.33	0/7919	0.61	0/10733
1	C	0.34	0/7911	0.63	3/10721 (0.0%)
1	D	0.35	0/7927	0.62	0/10744
All	All	0.34	0/31668	0.62	7/42919 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1017	LEU	N-CA-C	7.26	130.59	111.00
1	A	172	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	C	1017	LEU	CA-CB-CG	-6.20	101.03	115.30
1	A	905	PRO	N-CA-C	5.18	125.56	112.10
1	C	305	THR	N-CA-C	-5.06	97.33	111.00
1	A	1017	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	375	GLU	OE1-CD-OE2	5.04	129.35	123.30

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	7750	0	7775	179	0
1	B	7757	0	7782	136	1
1	C	7750	0	7775	185	0
1	D	7765	0	7793	173	1
2	A	32	0	0	1	0
2	B	32	0	0	2	0
2	C	32	0	0	1	0
2	D	32	0	0	2	0
3	A	31	0	19	1	0
3	B	31	0	19	1	0
3	C	31	0	19	0	0
3	D	31	0	19	0	0
4	A	53	0	31	2	0
4	B	53	0	31	2	0
4	C	53	0	31	2	0
4	D	53	0	31	2	0
5	A	1148	0	0	38	0
5	B	1125	0	0	34	0
5	C	1176	0	0	39	0
5	D	1190	0	0	41	0
All	All	36125	0	31325	607	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 10.

All (607) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ARG:HD2	5:A:2301:HOH:O	1.29	1.28
1:C:427:VAL:HG13	1:D:410:ARG:CZ	1.78	1.12
1:A:373:VAL:HB	5:A:2254:HOH:O	1.57	1.02
1:C:427:VAL:HG13	1:D:410:ARG:NH1	1.75	1.01
1:C:579:ASP:O	1:C:582:ILE:HG12	1.68	0.93
1:A:410:ARG:NH1	1:B:427:VAL:HG13	1.84	0.93
1:D:682:LEU:HA	5:D:2899:HOH:O	1.70	0.89
1:A:1017:LEU:O	5:A:3139:HOH:O	1.89	0.89
1:A:164:LYS:HG3	1:A:909:ARG:HH21	1.38	0.88
1:D:892:GLU:HG3	5:D:3065:HOH:O	1.72	0.88
1:D:51:HIS:HA	1:D:384:LYS:HG3	1.55	0.88
1:C:1017:LEU:HB3	5:C:2546:HOH:O	1.73	0.87
1:D:892:GLU:CG	5:D:3065:HOH:O	2.21	0.87
1:A:923:ASP:OD1	1:D:937:GLU:HG2	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:859:HIS:HD2	1:C:862:GLY:H	1.21	0.85
1:D:410:ARG:NH1	1:D:425:GLN:OE1	2.12	0.83
1:C:11:ASP:HB3	5:C:2028:HOH:O	1.78	0.83
1:D:856:THR:HG22	5:D:2184:HOH:O	1.78	0.82
1:D:867:ARG:HG3	1:D:872:MET:HE3	1.62	0.81
1:C:485:MET:HG2	1:D:35:LYS:HE3	1.62	0.80
1:C:343:THR:HA	4:C:1031:FAD:HM73	1.63	0.80
1:D:54:LYS:HE3	1:D:56:GLU:HB2	1.64	0.79
1:B:455:LYS:HD2	5:B:2618:HOH:O	1.81	0.79
1:A:427:VAL:CG2	1:B:410:ARG:CZ	2.61	0.79
1:C:893:GLU:OE1	1:C:896:ARG:NH2	2.16	0.78
1:D:867:ARG:HG3	1:D:872:MET:CE	2.13	0.78
1:C:53:GLU:OE2	1:C:55:LEU:HD21	1.84	0.78
1:A:375:GLU:OE1	1:A:375:GLU:N	2.16	0.77
1:C:428:HIS:N	1:D:410:ARG:HH12	1.83	0.77
1:A:722:ARG:O	1:A:726:GLU:HG3	1.85	0.76
1:A:1016:GLY:C	1:A:1017:LEU:HG	2.06	0.76
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.68	0.76
1:D:343:THR:HA	4:D:1031:FAD:HM73	1.69	0.76
1:D:682:LEU:HD23	5:D:2899:HOH:O	1.86	0.75
1:C:177:PRO:HG2	1:C:182:MET:SD	2.26	0.75
1:D:54:LYS:HE3	1:D:56:GLU:CB	2.17	0.75
1:A:373:VAL:CG1	5:A:2254:HOH:O	2.35	0.75
1:B:343:THR:HA	4:B:1031:FAD:HM73	1.67	0.75
1:C:164:LYS:O	1:C:909:ARG:NH2	2.21	0.74
1:C:410:ARG:CZ	1:D:427:VAL:HG22	2.17	0.74
1:A:343:THR:HA	4:A:1031:FAD:HM73	1.69	0.73
1:D:984:ASP:HB3	5:D:3145:HOH:O	1.86	0.73
1:D:896:ARG:O	1:D:900:GLN:HG3	1.87	0.73
1:D:173:ASN:HB2	5:D:2372:HOH:O	1.89	0.73
1:D:442:LEU:HD22	1:D:482:ILE:HD11	1.72	0.72
1:C:692:ARG:O	1:C:696:ARG:HG3	1.90	0.71
1:A:25:HIS:CD2	1:B:520:GLU:HG3	2.24	0.71
1:C:634:ASP:OD1	5:C:2793:HOH:O	2.07	0.71
1:D:53:GLU:HG3	1:D:887:LYS:HB3	1.71	0.71
1:B:673:HIS:CE1	1:B:682:LEU:HA	2.26	0.71
1:D:934:THR:OG1	1:D:937:GLU:HG3	1.91	0.71
1:D:1017:LEU:O	5:D:3179:HOH:O	2.08	0.71
1:A:427:VAL:CG2	1:B:410:ARG:NH2	2.54	0.70
1:A:410:ARG:CZ	1:B:427:VAL:HG13	2.21	0.70
1:C:680:MET:HE2	1:C:688:PRO:HD2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:950:GLU:HG3	1:D:979:LEU:HD22	1.74	0.70
1:C:859:HIS:CD2	1:C:862:GLY:H	2.08	0.69
1:D:722:ARG:O	1:D:726:GLU:HG3	1.93	0.69
1:A:1016:GLY:O	1:A:1017:LEU:HG	1.91	0.69
1:C:427:VAL:CG1	1:D:410:ARG:CZ	2.66	0.69
1:C:776:ARG:O	1:C:780:THR:HG23	1.93	0.69
1:D:173:ASN:HB3	1:D:176:LEU:HG	1.75	0.69
1:C:316:SER:HA	1:C:325:HIS:CD2	2.27	0.69
1:C:2:ALA:N	5:C:2002:HOH:O	2.26	0.69
1:C:9:VAL:HG23	1:C:11:ASP:OD1	1.93	0.69
1:D:885:GLN:HG3	5:D:3057:HOH:O	1.93	0.69
1:C:910:LYS:HE2	5:C:3032:HOH:O	1.93	0.69
1:D:9:VAL:HG23	1:D:11:ASP:OD1	1.93	0.68
1:C:680:MET:CE	1:C:688:PRO:HD2	2.23	0.68
1:A:856:THR:HA	5:A:2973:HOH:O	1.92	0.68
1:C:164:LYS:HG3	1:C:909:ARG:HH12	1.59	0.68
5:C:2780:HOH:O	1:D:2:ALA:HB3	1.94	0.67
1:C:36:LEU:HD22	5:C:2093:HOH:O	1.93	0.67
1:C:427:VAL:CG1	1:D:410:ARG:NH1	2.55	0.67
1:C:2:ALA:HB3	5:C:2001:HOH:O	1.94	0.67
1:A:12:ILE:O	1:A:15:ILE:HG22	1.93	0.67
1:C:143:TYR:O	1:D:861:LYS:HE3	1.93	0.67
1:C:428:HIS:H	1:D:410:ARG:NH1	1.93	0.66
1:B:259:LYS:HE2	5:B:2415:HOH:O	1.96	0.66
1:C:950:GLU:OE2	1:C:979:LEU:HD13	1.95	0.66
1:A:427:VAL:HG21	1:B:410:ARG:CZ	2.25	0.66
1:A:692:ARG:O	1:A:696:ARG:HG3	1.94	0.66
1:C:950:GLU:HG3	1:C:979:LEU:HD22	1.78	0.66
1:A:915:LYS:O	1:C:675:MET:HB2	1.95	0.66
1:D:1008:THR:HG22	5:D:3166:HOH:O	1.94	0.65
1:B:169:PRO:HG3	1:B:911:PRO:HB3	1.76	0.65
1:C:260:SER:HB2	1:C:265:GLU:OE1	1.95	0.65
1:C:12:ILE:O	1:C:15:ILE:HG22	1.96	0.65
1:A:718:VAL:CG2	1:A:780:THR:HG22	2.26	0.65
1:D:414:ASP:O	1:D:416:THR:N	2.29	0.65
1:A:5:LEU:HD22	1:A:1017:LEU:HD12	1.77	0.65
1:B:343:THR:HG21	5:B:2602:HOH:O	1.96	0.65
1:D:54:LYS:CE	1:D:56:GLU:HB3	2.27	0.65
1:D:1017:LEU:HB3	1:D:1018:PRO:CD	2.26	0.65
1:A:5:LEU:CD2	1:A:1017:LEU:HD12	2.27	0.65
1:B:173:ASN:HB2	5:B:2297:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:GLU:O	1:D:264:ASN:HB3	1.97	0.65
1:C:909:ARG:HG3	5:C:2283:HOH:O	1.96	0.64
1:B:442:LEU:HD22	1:B:482:ILE:HD11	1.79	0.64
1:C:486:ALA:HB3	5:C:2658:HOH:O	1.98	0.64
1:A:483:VAL:HG23	5:A:2663:HOH:O	1.97	0.64
1:A:261:LEU:HD21	1:A:451:LEU:HD21	1.81	0.63
1:A:1016:GLY:O	1:A:1017:LEU:CG	2.46	0.63
1:A:427:VAL:HG22	1:B:410:ARG:CZ	2.27	0.63
1:C:1017:LEU:CB	5:C:2546:HOH:O	2.35	0.63
1:B:722:ARG:O	1:B:726:GLU:HG3	1.98	0.63
1:C:428:HIS:N	1:D:410:ARG:NH1	2.46	0.63
1:A:173:ASN:HD22	1:A:174:PRO:CD	2.12	0.63
1:C:343:THR:HG21	5:C:2599:HOH:O	1.98	0.63
1:B:12:ILE:O	1:B:15:ILE:HG22	1.99	0.62
1:A:281:ILE:HD13	1:A:451:LEU:HD22	1.82	0.62
1:C:1015:ARG:HB2	1:C:1017:LEU:HG	1.80	0.62
1:A:263:GLU:O	1:A:264:ASN:HB2	1.98	0.62
1:A:293:ILE:CD1	1:A:393:PRO:HB2	2.29	0.62
1:A:293:ILE:HD11	1:A:393:PRO:HB2	1.82	0.62
1:D:897:LEU:HD23	1:D:900:GLN:OE1	2.00	0.62
1:B:173:ASN:HB3	1:B:176:LEU:HG	1.81	0.62
1:C:922:LYS:HE3	5:C:3051:HOH:O	2.00	0.61
1:C:410:ARG:NH2	1:D:427:VAL:CG2	2.63	0.61
1:C:978:HIS:HE1	1:D:84:ASP:OD2	1.83	0.61
1:C:410:ARG:HG3	1:C:425:GLN:HB3	1.83	0.61
1:C:877:PRO:HD2	1:C:882:TYR:CG	2.36	0.61
1:D:219:LYS:HG3	1:D:260:SER:OG	2.00	0.61
1:C:293:ILE:HD11	1:C:393:PRO:HB2	1.82	0.61
1:C:688:PRO:HG3	1:C:720:ILE:HD13	1.82	0.61
1:A:990:THR:O	1:A:990:THR:HG22	2.00	0.61
1:B:857:GLU:O	1:B:859:HIS:HD2	1.84	0.61
1:D:54:LYS:CE	1:D:56:GLU:CB	2.78	0.60
1:D:688:PRO:HG3	1:D:720:ILE:HD13	1.83	0.60
1:A:745:LYS:HD2	5:A:2886:HOH:O	2.01	0.60
1:C:22:THR:HG22	5:D:2238:HOH:O	2.02	0.60
1:A:173:ASN:HD22	1:A:174:PRO:N	1.99	0.60
1:A:699:ARG:O	1:A:699:ARG:HD3	2.02	0.60
1:A:787:GLY:HA3	1:D:942:GLU:OE2	2.01	0.60
1:A:1014:LYS:HB3	5:A:3138:HOH:O	1.99	0.60
1:B:411:THR:HG22	1:B:421:GLU:OE1	2.02	0.59
1:C:394:ARG:HH12	1:C:423:GLU:CD	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HG3	1:A:260:SER:OG	2.02	0.59
1:A:373:VAL:CB	5:A:2254:HOH:O	2.27	0.59
1:D:866:PRO:O	1:D:868:ILE:N	2.35	0.59
1:A:448:LYS:HD3	5:A:2611:HOH:O	2.01	0.59
1:A:911:PRO:HG2	5:A:2407:HOH:O	2.02	0.59
1:C:1017:LEU:HD11	5:D:2379:HOH:O	2.03	0.58
1:B:53:GLU:HG2	5:B:2124:HOH:O	2.02	0.58
1:D:990:THR:HG22	1:D:990:THR:O	2.02	0.58
1:C:844:GLU:O	1:C:847:GLN:HG3	2.02	0.58
1:A:900:GLN:HG2	1:A:900:GLN:O	2.03	0.58
1:C:990:THR:O	1:C:990:THR:HG22	2.02	0.58
1:C:783:ARG:HH11	1:C:932:LEU:HB3	1.68	0.58
1:C:716:ASP:OD2	1:C:719:SER:HB3	2.03	0.58
1:C:410:ARG:CZ	1:D:427:VAL:CG2	2.81	0.58
1:B:744:LEU:HD21	5:B:2430:HOH:O	2.03	0.58
1:D:923:ASP:O	1:D:927:LYS:HE3	2.04	0.58
1:B:410:ARG:HG3	1:B:425:GLN:HB3	1.85	0.58
1:C:173:ASN:OD1	1:C:174:PRO:HD2	2.04	0.58
1:A:12:ILE:HA	1:A:15:ILE:HG22	1.86	0.58
1:C:875:LYS:HA	1:C:950:GLU:OE2	2.04	0.58
1:A:427:VAL:HG21	1:B:410:ARG:NH2	2.19	0.57
1:C:722:ARG:O	1:C:726:GLU:HG3	2.04	0.57
1:C:410:ARG:NH1	5:C:2580:HOH:O	2.37	0.57
1:C:935:PHE:CE2	1:D:612:LEU:HD11	2.39	0.57
1:A:775:LEU:O	1:A:779:THR:HG23	2.05	0.57
1:A:410:ARG:NH1	1:A:425:GLN:OE1	2.28	0.57
1:A:416:THR:C	1:A:418:LYS:H	2.07	0.57
1:A:410:ARG:NH1	1:B:427:VAL:CG1	2.64	0.57
1:C:845:GLU:HG3	1:C:912:PHE:CE1	2.39	0.57
1:D:486:ALA:HB3	5:D:2715:HOH:O	2.04	0.57
1:A:173:ASN:HD22	1:A:174:PRO:HD2	1.69	0.57
1:B:326:SER:HB3	5:B:2486:HOH:O	2.04	0.57
1:C:50:PHE:HD1	5:C:2116:HOH:O	1.88	0.57
1:C:36:LEU:HG	5:C:2086:HOH:O	2.05	0.56
1:B:2:ALA:HB3	5:B:2001:HOH:O	2.03	0.56
1:B:866:PRO:HG3	5:B:2962:HOH:O	2.05	0.56
1:A:703:GLN:HG3	5:A:2851:HOH:O	2.04	0.56
1:A:22:THR:HG22	5:B:2211:HOH:O	2.04	0.56
1:D:54:LYS:HE2	1:D:56:GLU:HB3	1.87	0.56
1:C:293:ILE:CD1	1:C:393:PRO:HB2	2.36	0.56
1:B:907:LEU:O	1:B:909:ARG:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LEU:HD21	1:B:451:LEU:HD21	1.88	0.56
1:D:845:GLU:HG3	1:D:912:PHE:CE1	2.40	0.56
1:A:866:PRO:HG3	5:A:2142:HOH:O	2.05	0.55
1:C:892:GLU:HG3	5:C:3025:HOH:O	2.07	0.55
1:C:410:ARG:HG3	1:C:425:GLN:CB	2.37	0.55
1:A:307:LYS:HE3	5:A:2481:HOH:O	2.05	0.55
1:C:1015:ARG:C	1:C:1017:LEU:H	2.10	0.55
1:A:173:ASN:HD22	1:A:173:ASN:C	2.10	0.55
1:C:642:MET:HE2	5:C:2797:HOH:O	2.06	0.55
1:C:758:LYS:NZ	5:C:2900:HOH:O	2.38	0.55
1:A:834:LEU:HD21	1:A:921:ILE:HD11	1.88	0.55
1:A:29:HIS:HB2	5:B:2197:HOH:O	2.07	0.55
1:D:379:LEU:O	1:D:383:GLU:HG3	2.07	0.55
1:C:780:THR:HG22	1:D:762:TYR:CZ	2.41	0.54
1:A:179:GLN:HG3	5:A:2309:HOH:O	2.07	0.54
1:A:646:ASN:HD22	1:A:649:ASP:CG	2.10	0.54
1:C:612:LEU:HD11	1:D:935:PHE:CE2	2.43	0.54
1:A:779:THR:HG22	1:A:808:SER:HB3	1.89	0.54
1:C:505:LYS:HE2	5:C:2664:HOH:O	2.07	0.54
1:C:219:LYS:HG3	1:C:260:SER:OG	2.06	0.54
5:C:2196:HOH:O	1:D:29:HIS:HB2	2.07	0.54
1:B:293:ILE:CD1	1:B:393:PRO:HB2	2.37	0.54
1:D:307:LYS:HE3	5:D:2530:HOH:O	2.07	0.54
1:A:173:ASN:HB2	5:A:2347:HOH:O	2.08	0.54
1:C:711:THR:HG22	5:C:2843:HOH:O	2.07	0.54
1:C:783:ARG:NH1	1:C:932:LEU:HB3	2.22	0.54
1:B:990:THR:O	1:B:990:THR:HG22	2.07	0.54
1:A:646:ASN:ND2	1:A:649:ASP:H	2.06	0.53
1:A:688:PRO:HG3	1:A:720:ILE:HD13	1.88	0.53
1:D:53:GLU:HG3	1:D:887:LYS:CB	2.37	0.53
1:D:680:MET:CE	1:D:688:PRO:HD2	2.39	0.53
1:A:779:THR:HG21	5:A:2931:HOH:O	2.07	0.53
1:B:1012:GLU:HG2	5:B:3108:HOH:O	2.07	0.53
1:D:674:GLY:HA2	5:D:2901:HOH:O	2.08	0.53
1:C:868:ILE:HG22	1:C:870:GLU:H	1.73	0.53
1:C:27:ALA:O	1:D:497:LYS:HE2	2.08	0.53
1:C:287:GLU:OE2	1:C:444:ASP:HB2	2.07	0.53
1:A:15:ILE:HD13	1:A:969:GLN:O	2.08	0.53
1:B:691:VAL:HG21	1:B:720:ILE:HG23	1.90	0.53
1:B:849:TRP:CH2	1:B:854:PRO:HG3	2.44	0.53
1:C:179:GLN:HG3	5:C:2301:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:845:GLU:HG3	1:C:912:PHE:CD1	2.43	0.53
1:C:796:ILE:HD13	1:C:813:LEU:HB3	1.91	0.53
1:A:776:ARG:HB2	1:B:740:GLY:HA2	1.89	0.53
1:C:410:ARG:HB2	1:C:422:ASP:HB2	1.90	0.52
1:B:173:ASN:O	1:B:176:LEU:HB2	2.08	0.52
1:C:261:LEU:HD21	1:C:451:LEU:HD21	1.91	0.52
1:B:923:ASP:O	1:B:927:LYS:HE3	2.09	0.52
1:C:410:ARG:NH2	1:D:427:VAL:HG22	2.24	0.52
1:D:82:CYS:O	1:D:98:LYS:HD2	2.08	0.52
1:B:455:LYS:HD3	1:B:463:GLU:OE1	2.09	0.52
1:D:845:GLU:HG3	1:D:912:PHE:CD1	2.45	0.52
1:B:82:CYS:O	1:B:98:LYS:HD2	2.09	0.52
1:A:845:GLU:HG3	1:A:912:PHE:CE1	2.45	0.52
1:B:699:ARG:NE	1:B:699:ARG:HA	2.24	0.52
1:C:423:GLU:OE1	1:C:423:GLU:HA	2.09	0.52
1:B:173:ASN:ND2	5:B:2298:HOH:O	2.37	0.52
1:C:1017:LEU:CD1	5:D:2379:HOH:O	2.58	0.52
1:C:22:THR:HA	5:C:2063:HOH:O	2.10	0.52
1:A:46:ASP:HB3	1:A:49:CYS:SG	2.49	0.52
1:D:907:LEU:O	1:D:908:GLU:C	2.48	0.52
1:C:582:ILE:CD1	1:D:1019:LEU:HD21	2.40	0.52
1:C:691:VAL:HG21	1:C:720:ILE:HG23	1.92	0.51
1:A:172:ARG:HG3	5:A:2343:HOH:O	2.11	0.51
1:A:541:LYS:HD2	5:A:2715:HOH:O	2.10	0.51
1:D:263:GLU:OE1	1:D:263:GLU:HA	2.11	0.51
1:C:82:CYS:O	1:C:98:LYS:HD2	2.11	0.51
1:A:796:ILE:HD13	1:A:813:LEU:HB3	1.93	0.51
1:D:263:GLU:O	1:D:264:ASN:CB	2.59	0.51
1:C:955:ASN:HB3	1:C:978:HIS:HB3	1.92	0.51
1:D:909:ARG:NH2	5:D:3071:HOH:O	2.43	0.51
1:A:955:ASN:HB3	1:A:978:HIS:HB3	1.91	0.51
1:A:874:LYS:NZ	5:A:2994:HOH:O	2.42	0.51
1:C:978:HIS:HD2	5:D:2284:HOH:O	1.94	0.51
1:A:288:PRO:HG3	1:A:307:LYS:HB2	1.92	0.51
1:B:892:GLU:HG3	5:B:2981:HOH:O	2.11	0.51
1:A:39:LYS:NZ	5:A:2102:HOH:O	2.43	0.51
1:B:173:ASN:HB3	1:B:176:LEU:CG	2.40	0.51
1:A:705:PRO:HA	1:A:730:ASP:OD2	2.11	0.50
1:B:1014:LYS:HE3	5:B:3058:HOH:O	2.11	0.50
1:C:1014:LYS:NZ	5:C:3164:HOH:O	2.32	0.50
1:C:410:ARG:HH22	1:D:391:LEU:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:CYS:HB2	5:B:2300:HOH:O	2.11	0.50
1:C:394:ARG:NH2	1:C:423:GLU:OE2	2.38	0.50
1:A:725:LYS:HE3	5:A:2917:HOH:O	2.11	0.50
1:D:796:ILE:HD13	1:D:813:LEU:HB3	1.93	0.50
1:B:191:ALA:O	1:B:279:ALA:HA	2.12	0.50
1:C:758:LYS:HD3	5:C:2902:HOH:O	2.11	0.50
1:B:358:ARG:NH2	5:B:2544:HOH:O	2.40	0.50
1:A:935:PHE:CE2	1:B:612:LEU:HD11	2.47	0.50
1:B:915:LYS:HG3	5:B:2933:HOH:O	2.10	0.50
1:C:52:CYS:HB2	1:C:384:LYS:HB2	1.93	0.50
1:A:82:CYS:O	1:A:98:LYS:HD2	2.12	0.50
1:C:893:GLU:HA	1:C:896:ARG:HH21	1.77	0.50
1:C:497:LYS:HE2	1:D:27:ALA:O	2.12	0.50
1:A:53:GLU:OE2	1:A:55:LEU:HD21	2.11	0.50
1:C:1014:LYS:HB3	5:C:3167:HOH:O	2.12	0.50
1:B:845:GLU:HG3	1:B:912:PHE:CE1	2.46	0.50
1:D:682:LEU:CD2	5:D:2899:HOH:O	2.54	0.49
1:B:346:ASP:OD2	4:B:1031:FAD:H6	2.12	0.49
1:A:572:LEU:HD13	1:A:638:ILE:HB	1.93	0.49
1:C:442:LEU:HD22	1:C:482:ILE:CD1	2.40	0.49
1:A:35:LYS:NZ	5:A:2092:HOH:O	2.44	0.49
1:C:364:ARG:NH1	5:C:2586:HOH:O	2.44	0.49
1:A:97:ILE:HA	1:A:100:PHE:CD2	2.47	0.49
1:B:870:GLU:N	1:B:870:GLU:OE1	2.44	0.49
1:A:386:GLU:HA	5:A:2574:HOH:O	2.12	0.49
1:A:672:PRO:HA	1:A:682:LEU:O	2.13	0.49
1:A:909:ARG:NH1	5:A:3022:HOH:O	2.46	0.49
1:A:868:ILE:O	1:A:872:MET:HG2	2.13	0.49
1:B:442:LEU:HD22	1:B:482:ILE:CD1	2.42	0.49
1:B:193:LEU:N	1:B:193:LEU:HD22	2.28	0.49
1:A:413:GLN:CG	1:A:417:GLY:HA2	2.42	0.49
1:C:410:ARG:HD2	5:C:2579:HOH:O	2.13	0.49
1:B:430:LYS:HE2	5:B:2594:HOH:O	2.11	0.49
1:A:845:GLU:HG3	1:A:912:PHE:CD1	2.48	0.49
1:A:346:ASP:OD2	4:A:1031:FAD:H6	2.13	0.49
1:B:621:TRP:O	1:B:625:VAL:HG23	2.12	0.49
1:B:410:ARG:HG3	1:B:425:GLN:CB	2.42	0.49
1:A:281:ILE:HD13	1:A:451:LEU:CD2	2.42	0.49
1:A:699:ARG:NH2	1:A:730:ASP:OD2	2.46	0.49
1:A:95:LEU:HD12	1:A:119:ASP:HB2	1.95	0.49
1:D:896:ARG:C	1:D:900:GLN:HG3	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:673:HIS:O	1:C:674:GLY:O	2.30	0.48
1:D:346:ASP:OD2	4:D:1031:FAD:H6	2.12	0.48
1:C:407:GLN:NE2	5:C:2577:HOH:O	2.47	0.48
1:D:959:CYS:O	1:D:962:THR:HG22	2.12	0.48
1:A:379:LEU:O	1:A:383:GLU:HG3	2.13	0.48
1:B:219:LYS:HG3	1:B:260:SER:OG	2.12	0.48
1:A:427:VAL:HG22	1:B:410:ARG:NE	2.27	0.48
1:C:779:THR:HG22	1:C:808:SER:HB3	1.95	0.48
5:A:2209:HOH:O	1:B:29:HIS:HB2	2.12	0.48
1:C:412:GLU:OE1	1:C:422:ASP:OD2	2.31	0.48
1:C:418:LYS:HE2	1:C:420:ASN:OD1	2.14	0.48
1:C:246:GLU:OE1	1:C:908:GLU:OE1	2.32	0.48
1:D:451:LEU:O	1:D:454:ILE:HG12	2.14	0.48
1:D:933:GLY:HA3	1:D:937:GLU:OE1	2.14	0.48
1:C:859:HIS:HA	1:C:865:VAL:HG23	1.96	0.48
1:C:780:THR:HG22	1:D:762:TYR:CE2	2.48	0.48
1:C:394:ARG:NH2	1:C:421:GLU:OE1	2.47	0.48
1:C:760:THR:CG2	1:D:932:LEU:HD23	2.44	0.48
1:D:758:LYS:HD3	5:D:2948:HOH:O	2.13	0.48
1:C:331:ILE:HG23	1:C:433:VAL:HG21	1.95	0.48
1:B:796:ILE:HD13	1:B:813:LEU:HB3	1.95	0.48
1:C:346:ASP:OD2	4:C:1031:FAD:H6	2.13	0.48
1:B:845:GLU:HG3	1:B:912:PHE:CD1	2.48	0.48
1:A:582:ILE:HD11	1:B:1015:ARG:CZ	2.43	0.48
1:C:47:LYS:HD3	1:D:373:VAL:HG12	1.96	0.48
1:C:167:ASN:OD1	1:C:909:ARG:NE	2.38	0.48
1:D:193:LEU:HD22	1:D:193:LEU:N	2.28	0.48
1:D:458:ARG:HH21	1:D:459:TRP:HH2	1.62	0.48
1:B:859:HIS:CE1	1:B:864:PRO:HG3	2.48	0.48
1:C:191:ALA:O	1:C:279:ALA:HA	2.14	0.48
1:D:97:ILE:HD11	2:D:1026:SF4:S2	2.53	0.48
1:B:520:GLU:OE1	5:B:2674:HOH:O	2.20	0.47
1:D:950:GLU:OE2	1:D:979:LEU:HD13	2.14	0.47
1:D:673:HIS:HD2	1:D:675:MET:H	1.61	0.47
1:A:387:PHE:HD1	5:A:2574:HOH:O	1.97	0.47
1:B:291:ASP:OD1	1:B:293:ILE:HG12	2.13	0.47
1:B:1014:LYS:HB3	5:B:3114:HOH:O	2.15	0.47
1:C:364:ARG:CZ	5:C:2586:HOH:O	2.62	0.47
1:C:861:LYS:HE3	5:D:2286:HOH:O	2.13	0.47
1:B:688:PRO:HG3	1:B:720:ILE:HD13	1.96	0.47
1:B:5:LEU:HD21	1:B:1017:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:GLU:O	1:B:55:LEU:HG	2.14	0.47
1:D:892:GLU:HG3	5:D:3063:HOH:O	2.15	0.47
1:C:859:HIS:HD2	1:C:862:GLY:N	2.00	0.47
1:C:193:LEU:HD22	1:C:193:LEU:N	2.30	0.47
1:C:394:ARG:HD3	1:C:394:ARG:HA	1.68	0.47
1:C:870:GLU:OE1	1:C:889:ILE:HG23	2.14	0.47
1:B:1017:LEU:HB3	1:B:1018:PRO:CD	2.45	0.47
1:C:2:ALA:HB3	5:D:2832:HOH:O	2.14	0.47
1:D:680:MET:HE1	1:D:688:PRO:HD2	1.95	0.46
1:A:691:VAL:HG21	1:A:720:ILE:HG23	1.97	0.46
1:A:776:ARG:HD2	1:B:739:SER:OG	2.15	0.46
1:D:908:GLU:O	1:D:910:LYS:HG2	2.15	0.46
1:D:468:THR:HA	1:D:502:TYR:CD2	2.50	0.46
1:D:621:TRP:O	1:D:625:VAL:HG23	2.15	0.46
1:A:193:LEU:N	1:A:193:LEU:HD22	2.30	0.46
1:A:143:TYR:O	1:B:861:LYS:HE2	2.14	0.46
1:D:892:GLU:HG2	5:D:3065:HOH:O	2.01	0.46
1:B:870:GLU:O	1:B:889:ILE:HD13	2.15	0.46
1:D:2:ALA:HB1	1:D:3:PRO:HD2	1.98	0.46
1:A:413:GLN:HE21	1:A:417:GLY:CA	2.28	0.46
1:A:116:ILE:HD13	1:A:156:GLN:HG3	1.97	0.46
1:C:519:PRO:HB3	1:D:28:LEU:HD22	1.97	0.46
1:D:552:ALA:HB3	1:D:553:PRO:HD3	1.96	0.46
1:D:371:ARG:NH1	5:D:2615:HOH:O	2.49	0.46
1:D:2:ALA:HB3	5:D:2001:HOH:O	2.14	0.46
1:B:955:ASN:HB3	1:B:978:HIS:HB3	1.97	0.46
1:D:672:PRO:HA	1:D:682:LEU:O	2.15	0.46
1:C:984:ASP:CG	5:C:3153:HOH:O	2.53	0.46
1:A:173:ASN:ND2	1:A:173:ASN:C	2.67	0.46
1:B:486:ALA:HB1	1:B:491:GLU:OE1	2.15	0.46
1:C:368:VAL:HG11	1:D:50:PHE:O	2.16	0.46
1:A:892:GLU:HG3	5:A:3013:HOH:O	2.14	0.46
1:B:572:LEU:HD13	1:B:638:ILE:HB	1.97	0.46
1:A:131:PRO:HB2	1:A:373:VAL:HG11	1.98	0.46
1:D:173:ASN:O	1:D:176:LEU:HB2	2.15	0.46
1:D:486:ALA:HB1	1:D:491:GLU:OE1	2.16	0.46
1:B:7:LYS:NZ	5:B:2017:HOH:O	2.41	0.46
1:C:705:PRO:HA	1:C:730:ASP:OD2	2.15	0.46
1:C:849:TRP:CH2	1:C:854:PRO:HG3	2.51	0.46
1:D:574:LYS:HG3	1:D:614:SER:HB2	1.98	0.46
1:A:622:CYS:SG	1:A:656:LYS:HD2	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:GLU:OE1	1:B:375:GLU:HA	2.16	0.46
1:D:53:GLU:HG3	1:D:887:LYS:HD3	1.98	0.45
1:A:263:GLU:O	1:A:264:ASN:CB	2.64	0.45
1:A:486:ALA:HB1	1:A:491:GLU:OE1	2.15	0.45
1:A:164:LYS:O	1:A:909:ARG:NH2	2.47	0.45
1:C:393:PRO:HD3	5:C:2562:HOH:O	2.15	0.45
1:D:955:ASN:HB3	1:D:978:HIS:HB3	1.97	0.45
1:D:394:ARG:HG2	1:D:394:ARG:HH11	1.80	0.45
1:B:307:LYS:HE3	5:B:2482:HOH:O	2.16	0.45
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.98	0.45
1:B:896:ARG:NH2	5:B:2985:HOH:O	2.48	0.45
1:C:876:LEU:HD22	1:C:885:GLN:OE1	2.17	0.45
1:B:410:ARG:HB2	1:B:422:ASP:HB2	1.99	0.45
1:A:932:LEU:HD21	5:B:2430:HOH:O	2.16	0.45
1:D:100:PHE:C	1:D:100:PHE:CD1	2.90	0.45
1:D:293:ILE:CD1	1:D:393:PRO:HB2	2.46	0.45
1:D:871:LEU:HG	1:D:889:ILE:HG21	1.98	0.45
1:C:164:LYS:CG	1:C:909:ARG:HH12	2.29	0.45
5:A:2266:HOH:O	1:B:861:LYS:HE3	2.16	0.45
1:B:574:LYS:CG	1:B:614:SER:HB2	2.47	0.45
1:C:915:LYS:HG2	5:C:3037:HOH:O	2.16	0.45
1:D:191:ALA:O	1:D:279:ALA:HA	2.16	0.45
1:A:164:LYS:HG3	1:A:909:ARG:NH2	2.19	0.45
1:D:173:ASN:HA	1:D:174:PRO:HD3	1.86	0.45
1:A:281:ILE:CD1	1:A:451:LEU:HD22	2.46	0.45
1:D:291:ASP:OD1	1:D:293:ILE:HG12	2.16	0.45
1:B:577:SER:HB2	5:B:2718:HOH:O	2.15	0.45
1:D:328:LEU:HD12	5:D:2147:HOH:O	2.15	0.45
1:D:173:ASN:HB3	1:D:176:LEU:CG	2.44	0.45
1:B:293:ILE:HD11	1:B:393:PRO:HB2	1.99	0.45
1:C:1014:LYS:CE	5:C:3164:HOH:O	2.63	0.45
1:C:28:LEU:HD11	1:D:498:GLN:HA	1.99	0.45
1:B:705:PRO:HA	1:B:730:ASP:OD2	2.17	0.45
1:B:552:ALA:HB2	3:B:1030:FMN:HM73	1.99	0.45
1:A:89:LYS:HE2	5:B:2043:HOH:O	2.16	0.45
1:A:84:ASP:CG	1:A:89:LYS:NZ	2.71	0.45
1:A:480:GLY:O	1:A:483:VAL:HG22	2.17	0.44
1:A:173:ASN:OD1	5:A:2306:HOH:O	2.21	0.44
1:A:41:TRP:CE2	1:B:89:LYS:HD2	2.51	0.44
1:A:552:ALA:HB3	1:A:553:PRO:HD3	2.00	0.44
1:D:54:LYS:HG3	1:D:55:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:PRO:HD3	5:A:2578:HOH:O	2.16	0.44
1:A:710:LEU:HD22	1:A:720:ILE:HG22	2.00	0.44
1:A:870:GLU:O	1:A:874:LYS:HE3	2.17	0.44
1:A:413:GLN:HE21	1:A:417:GLY:HA2	1.82	0.44
1:D:993:LEU:HD23	1:D:993:LEU:C	2.38	0.44
1:A:416:THR:O	1:A:418:LYS:N	2.50	0.44
1:C:870:GLU:O	1:C:870:GLU:HG2	2.17	0.44
1:B:97:ILE:HA	1:B:100:PHE:CD2	2.53	0.44
1:A:828:GLN:NE2	5:A:2942:HOH:O	2.50	0.44
1:A:107:LYS:NZ	5:A:2231:HOH:O	2.50	0.44
1:C:410:ARG:NH2	1:D:427:VAL:HG21	2.33	0.44
1:B:2:ALA:HB1	1:B:3:PRO:HD2	2.00	0.44
1:C:97:ILE:HD11	2:C:1026:SF4:S2	2.58	0.44
1:B:364:ARG:HA	1:B:391:LEU:O	2.17	0.44
1:A:849:TRP:CH2	1:A:854:PRO:HG3	2.52	0.44
1:A:784:ALA:C	1:A:786:PRO:HD3	2.38	0.44
1:B:53:GLU:CG	5:B:2124:HOH:O	2.63	0.44
1:A:191:ALA:O	1:A:279:ALA:HA	2.17	0.44
1:C:621:TRP:O	1:C:625:VAL:HG23	2.18	0.44
1:A:917:PRO:HG3	1:C:675:MET:HE3	1.99	0.44
1:A:416:THR:C	1:A:418:LYS:N	2.71	0.44
1:D:395:LYS:HD3	5:D:2643:HOH:O	2.18	0.44
1:C:871:LEU:O	1:C:873:GLY:N	2.48	0.44
1:D:116:ILE:HD13	1:D:156:GLN:HG3	1.99	0.44
1:A:930:GLN:HB3	5:D:3100:HOH:O	2.16	0.44
1:D:572:LEU:HD13	1:D:638:ILE:HB	1.99	0.44
1:B:911:PRO:HG3	5:B:2133:HOH:O	2.17	0.43
1:C:845:GLU:HG3	1:C:912:PHE:CZ	2.53	0.43
1:C:888:LYS:HG2	1:C:892:GLU:OE2	2.18	0.43
1:C:870:GLU:O	1:C:889:ILE:HD13	2.18	0.43
1:C:29:HIS:HB2	5:D:2225:HOH:O	2.18	0.43
1:C:572:LEU:HD13	1:C:638:ILE:HB	1.99	0.43
1:B:140:CYS:HA	2:B:1027:SF4:S1	2.57	0.43
1:B:868:ILE:HG22	1:B:870:GLU:H	1.83	0.43
1:C:386:GLU:HB2	5:C:2526:HOH:O	2.18	0.43
1:C:427:VAL:HG13	1:D:410:ARG:NH2	2.27	0.43
1:A:89:LYS:HD2	1:B:41:TRP:CE2	2.53	0.43
1:A:394:ARG:HA	1:A:394:ARG:HD3	1.80	0.43
1:D:577:SER:HB2	5:D:2789:HOH:O	2.18	0.43
1:B:320:GLY:O	1:B:321:MET:C	2.56	0.43
1:D:898:LYS:HE2	5:D:2259:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:916:LYS:HD3	5:B:3002:HOH:O	2.17	0.43
1:B:779:THR:HG22	1:B:808:SER:HB3	2.00	0.43
1:C:1017:LEU:O	1:C:1017:LEU:HD22	2.18	0.43
1:A:480:GLY:O	1:A:483:VAL:CG2	2.66	0.43
1:D:868:ILE:HG22	1:D:870:GLU:H	1.83	0.43
1:B:413:GLN:HG3	1:B:417:GLY:O	2.18	0.43
1:D:691:VAL:HG21	1:D:720:ILE:HG23	1.99	0.43
1:B:541:LYS:HB3	5:B:2697:HOH:O	2.18	0.43
1:D:948:ILE:HG12	1:D:1002:ILE:HG12	1.99	0.43
1:D:54:LYS:CE	1:D:56:GLU:HB2	2.42	0.43
1:D:391:LEU:HD21	1:D:427:VAL:HG21	2.00	0.43
1:D:219:LYS:HE2	5:D:3188:HOH:O	2.19	0.43
1:D:298:THR:HB	5:D:2520:HOH:O	2.19	0.43
1:B:289:LYS:HG3	1:B:441:VAL:HG13	2.00	0.43
1:B:387:PHE:CD1	1:B:387:PHE:N	2.86	0.43
1:D:734:ALA:HA	1:D:735:THR:HA	1.61	0.43
1:A:740:GLY:HA2	1:B:776:ARG:HB2	1.99	0.43
1:C:191:ALA:HB2	1:C:276:TYR:CD2	2.54	0.43
1:D:297:LEU:HA	1:D:301:GLN:OE1	2.18	0.43
1:A:1015:ARG:CZ	1:B:582:ILE:HD11	2.49	0.43
1:A:909:ARG:NH1	5:A:3024:HOH:O	2.52	0.43
1:A:870:GLU:HG2	1:A:889:ILE:HD13	2.01	0.43
1:B:1009:THR:HB	1:B:1010:PRO:HD2	2.01	0.43
1:D:140:CYS:HA	2:D:1027:SF4:S1	2.59	0.43
1:A:44:ASN:HB2	1:A:45:PRO:CD	2.49	0.43
1:B:173:ASN:HB3	1:B:176:LEU:CD1	2.49	0.43
1:A:612:LEU:HD11	1:B:935:PHE:CE2	2.53	0.43
1:B:367:PHE:O	1:B:370:ILE:HG13	2.19	0.43
1:C:427:VAL:CG1	1:D:410:ARG:NH2	2.81	0.43
1:A:5:LEU:HG	1:B:623:GLN:NE2	2.34	0.43
1:D:867:ARG:HG3	1:D:872:MET:HE1	1.99	0.43
1:A:358:ARG:NH2	5:A:2535:HOH:O	2.51	0.42
1:C:116:ILE:HD13	1:C:156:GLN:HG3	2.01	0.42
1:B:734:ALA:HA	1:B:735:THR:HA	1.61	0.42
1:A:391:LEU:HD21	1:B:410:ARG:HH22	1.84	0.42
1:A:671:CYS:HA	1:A:672:PRO:HD3	1.80	0.42
1:A:574:LYS:CG	1:A:614:SER:HB2	2.48	0.42
1:B:834:LEU:HD21	1:B:921:ILE:HD11	2.00	0.42
1:C:993:LEU:HD23	1:C:993:LEU:C	2.40	0.42
1:A:1015:ARG:C	1:A:1017:LEU:H	2.22	0.42
1:C:173:ASN:HB2	5:C:2333:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:LYS:CE	1:B:143:TYR:O	2.68	0.42
1:C:309:PHE:CE1	1:C:331:ILE:HD11	2.55	0.42
1:D:849:TRP:CH2	1:D:854:PRO:HG3	2.54	0.42
1:A:124:LEU:HD13	1:A:160:SER:HB2	2.02	0.42
1:B:643:CYS:HB2	1:B:650:TRP:CE2	2.54	0.42
1:A:73:LEU:HD13	1:B:598:PRO:HB2	2.02	0.42
1:C:1015:ARG:C	1:C:1017:LEU:N	2.73	0.42
1:D:83:ALA:O	1:D:84:ASP:C	2.58	0.42
1:A:363:PHE:CZ	1:A:387:PHE:HD2	2.37	0.42
1:C:369:ASN:ND2	1:D:50:PHE:CD2	2.87	0.42
1:C:307:LYS:HE3	5:C:2474:HOH:O	2.20	0.42
1:C:574:LYS:CG	1:C:614:SER:HB2	2.49	0.42
1:D:249:LYS:NZ	5:D:2432:HOH:O	2.51	0.42
1:D:1017:LEU:HB3	1:D:1018:PRO:HD3	2.00	0.42
1:A:261:LEU:HD21	1:A:451:LEU:CD2	2.49	0.42
1:A:269:ASN:O	1:A:273:GLU:HB2	2.19	0.42
1:A:734:ALA:HA	1:A:735:THR:HA	1.62	0.42
1:D:705:PRO:HA	1:D:730:ASP:OD2	2.20	0.42
1:D:845:GLU:H	1:D:845:GLU:CD	2.22	0.42
1:B:169:PRO:HG3	1:B:911:PRO:CB	2.45	0.42
1:C:760:THR:HG22	1:D:932:LEU:HD23	2.01	0.42
1:A:552:ALA:HB2	3:A:1030:FMN:HM73	2.01	0.42
1:B:220:GLN:O	1:B:257:CYS:HB3	2.19	0.42
1:D:1015:ARG:HB2	5:D:3176:HOH:O	2.19	0.42
1:A:5:LEU:CD2	1:A:1017:LEU:CD1	2.97	0.42
1:A:291:ASP:OD1	1:A:293:ILE:HG12	2.19	0.42
1:A:622:CYS:SG	1:A:656:LYS:CD	3.08	0.42
1:A:394:ARG:NH2	1:A:421:GLU:OE1	2.52	0.42
1:B:44:ASN:HB2	1:B:45:PRO:CD	2.50	0.42
1:C:759:ARG:NH2	1:D:937:GLU:OE1	2.53	0.41
1:A:191:ALA:HB2	1:A:276:TYR:CD2	2.55	0.41
1:B:311:PRO:O	1:B:315:LYS:HG3	2.19	0.41
1:C:533:ILE:O	1:C:545:PRO:HD3	2.19	0.41
1:A:200:ILE:CD1	1:A:245:ILE:HD11	2.50	0.41
1:A:39:LYS:NZ	5:A:2103:HOH:O	2.52	0.41
1:D:97:ILE:HA	1:D:100:PHE:CD2	2.55	0.41
1:A:20:PRO:HG2	1:A:961:MET:SD	2.60	0.41
1:B:22:THR:HA	5:B:2056:HOH:O	2.20	0.41
1:C:20:PRO:HG2	1:C:961:MET:SD	2.60	0.41
1:B:948:ILE:HG12	1:B:1002:ILE:HG12	2.02	0.41
1:A:133:SER:OG	5:A:2254:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:LYS:NZ	1:D:460:ASP:OD2	2.45	0.41
1:A:845:GLU:HG3	1:A:912:PHE:CZ	2.55	0.41
1:A:771:ARG:N	1:A:772:PRO:CD	2.83	0.41
1:C:644:SER:HA	1:C:671:CYS:SG	2.61	0.41
1:A:394:ARG:HH11	1:A:394:ARG:HG3	1.85	0.41
1:A:549:ALA:HB2	1:A:814:GLN:HB3	2.03	0.41
1:A:204:SER:O	1:A:208:ARG:HG3	2.21	0.41
1:C:379:LEU:O	1:C:383:GLU:HG3	2.20	0.41
1:C:577:SER:HB2	5:C:2733:HOH:O	2.20	0.41
1:A:907:LEU:O	1:A:908:GLU:C	2.59	0.41
1:D:643:CYS:HB2	1:D:650:TRP:CE2	2.55	0.41
1:B:777:ALA:O	1:B:780:THR:HG22	2.20	0.41
1:C:100:PHE:C	1:C:100:PHE:CD1	2.93	0.41
1:C:97:ILE:HA	1:C:100:PHE:CD2	2.56	0.41
1:C:83:ALA:O	1:C:84:ASP:C	2.59	0.41
1:A:337:VAL:HB	1:A:361:LEU:HD23	2.02	0.41
1:B:901:ASN:OD1	1:B:902:ALA:N	2.53	0.41
1:D:968:TYR:N	1:D:968:TYR:CD1	2.88	0.41
1:C:901:ASN:C	1:C:901:ASN:OD1	2.59	0.41
1:D:533:ILE:O	1:D:545:PRO:HD3	2.20	0.41
1:D:449:GLU:HG2	5:D:2675:HOH:O	2.19	0.41
1:C:582:ILE:HD11	1:D:1019:LEU:HD21	2.02	0.41
1:D:9:VAL:CG2	1:D:11:ASP:OD1	2.67	0.41
1:C:486:ALA:HB1	1:C:491:GLU:OE1	2.21	0.41
1:D:261:LEU:HD21	1:D:451:LEU:HD21	2.03	0.41
1:B:771:ARG:N	1:B:772:PRO:CD	2.84	0.41
1:A:518:LYS:O	1:A:520:GLU:HG3	2.20	0.41
1:D:783:ARG:NE	5:D:2973:HOH:O	2.54	0.41
1:C:387:PHE:N	1:C:387:PHE:CD1	2.88	0.41
1:C:734:ALA:HA	1:C:735:THR:HA	1.66	0.41
1:A:140:CYS:HA	2:A:1027:SF4:S1	2.61	0.41
1:D:909:ARG:O	1:D:910:LYS:HD3	2.21	0.41
1:A:143:TYR:O	1:B:861:LYS:CE	2.69	0.41
1:B:106:ASN:O	1:B:107:LYS:HB2	2.21	0.41
1:D:335:VAL:HG22	1:D:433:VAL:HB	2.03	0.41
1:D:5:LEU:HD21	1:D:1017:LEU:HD21	2.03	0.40
1:D:950:GLU:CD	1:D:979:LEU:HD13	2.42	0.40
1:C:780:THR:HG22	1:D:762:TYR:OH	2.21	0.40
1:D:414:ASP:C	1:D:416:THR:H	2.24	0.40
1:D:191:ALA:HB2	1:D:276:TYR:CD2	2.56	0.40
1:D:647:LYS:O	1:D:651:MET:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:GLN:HG3	5:B:2306:HOH:O	2.21	0.40
1:A:497:LYS:HE2	1:B:27:ALA:O	2.21	0.40
1:C:394:ARG:NH1	1:C:423:GLU:OE2	2.53	0.40
1:C:779:THR:CG2	1:C:808:SER:HB3	2.51	0.40
1:D:521:LEU:HA	1:D:522:PRO:HD3	1.91	0.40
1:D:57:ASN:HB2	5:D:2147:HOH:O	2.20	0.40
1:B:97:ILE:HD11	2:B:1026:SF4:S2	2.61	0.40
1:C:44:ASN:HB2	1:C:45:PRO:CD	2.51	0.40
1:B:470:GLN:HG2	5:B:2633:HOH:O	2.22	0.40
1:D:39:LYS:HE2	5:D:2111:HOH:O	2.20	0.40
1:D:892:GLU:CA	5:D:3065:HOH:O	2.68	0.40
1:B:845:GLU:CD	1:B:845:GLU:H	2.23	0.40
1:B:552:ALA:HB3	1:B:553:PRO:HD3	2.03	0.40
1:A:84:ASP:CG	1:A:89:LYS:HZ1	2.25	0.40
1:C:131:PRO:HB2	1:C:373:VAL:HG11	2.03	0.40
1:A:1014:LYS:HE3	5:A:3082:HOH:O	2.21	0.40
1:C:521:LEU:O	1:D:25:HIS:HB3	2.21	0.40
1:B:116:ILE:HD13	1:B:156:GLN:HG3	2.03	0.40
1:A:310:LEU:HB2	1:A:311:PRO:HD3	2.04	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:B:460:ASP:OD1	1:D:395:LYS:NZ[1_656]	2.16	0.04

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	1014/1025 (99%)	974 (96%)	32 (3%)	8 (1%)	24 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	1015/1025 (99%)	967 (95%)	36 (4%)	12 (1%)	16 5
1	C	1014/1025 (99%)	970 (96%)	38 (4%)	6 (1%)	30 17
1	D	1016/1025 (99%)	972 (96%)	34 (3%)	10 (1%)	19 7
All	All	4059/4100 (99%)	3883 (96%)	140 (3%)	36 (1%)	21 9

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	904	PHE
1	A	908	GLU
1	B	675	MET
1	B	677	GLU
1	B	906	PRO
1	C	678	ARG
1	C	872	MET
1	D	415	GLU
1	D	867	ARG
1	D	903	ALA
1	D	906	PRO
1	D	1017	LEU
1	A	901	ASN
1	B	416	THR
1	B	903	ALA
1	B	908	GLU
1	C	414	ASP
1	C	674	GLY
1	D	676	GLY
1	A	907	LEU
1	B	3	PRO
1	B	321	MET
1	D	3	PRO
1	D	908	GLU
1	D	1018	PRO
1	A	417	GLY
1	A	678	ARG
1	B	905	PRO
1	C	680	MET
1	D	866	PRO
1	A	175	CYS
1	A	906	PRO
1	B	175	CYS

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Mol	Chain	Res	Type
1	B	676	GLY
1	C	3	PRO
1	B	904	PHE

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	846/854 (99%)	828 (98%)	18 (2%)	61	55
1	B	847/854 (99%)	837 (99%)	10 (1%)	78	76
1	C	846/854 (99%)	836 (99%)	10 (1%)	78	76
1	D	848/854 (99%)	843 (99%)	5 (1%)	90	90
All	All	3387/3416 (99%)	3344 (99%)	43 (1%)	76	73

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	100	PHE
1	A	133	SER
1	A	173	ASN
1	A	273	GLU
1	A	407	GLN
1	A	453	PRO
1	A	483	VAL
1	A	541	LYS
1	A	656	LYS
1	A	677	GLU
1	A	776	ARG
1	A	793	THR
1	A	800	GLU
1	A	906	PRO
1	A	932	LEU
1	A	955	ASN
1	A	1017	LEU

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Mol	Chain	Res	Type
1	B	95	LEU
1	B	100	PHE
1	B	273	GLU
1	B	394	ARG
1	B	443	ARG
1	B	453	PRO
1	B	675	MET
1	B	793	THR
1	B	828	GLN
1	B	907	LEU
1	C	100	PHE
1	C	184	GLU
1	C	259	LYS
1	C	326	SER
1	C	453	PRO
1	C	793	THR
1	C	800	GLU
1	C	896	ARG
1	C	955	ASN
1	C	1017	LEU
1	D	95	LEU
1	D	100	PHE
1	D	453	PRO
1	D	599	MET
1	D	800	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	295	GLN
1	A	407	GLN
1	A	413	GLN
1	A	646	ASN
1	B	295	GLN
1	B	703	GLN
1	B	859	HIS
1	C	295	GLN
1	C	407	GLN
1	C	859	HIS
1	C	978	HIS
1	D	48	ASN

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Mol	Chain	Res	Type
1	D	242	ASN
1	D	673	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

24 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	SF4	A	1026	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1027	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1028	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1029	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	A	1030	-	32,33,33	2.66	10 (31%)	34,50,50	3.64	12 (35%)
4	FAD	A	1031	-	52,58,58	2.13	19 (36%)	52,89,89	2.00	11 (21%)
2	SF4	B	1026	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1027	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1028	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1029	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	B	1030	-	32,33,33	2.58	10 (31%)	34,50,50	3.64	13 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FAD	B	1031	-	52,58,58	2.18	19 (36%)	52,89,89	2.00	11 (21%)
2	SF4	C	1026	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	1027	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	1028	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	1029	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	C	1030	-	32,33,33	2.71	10 (31%)	34,50,50	3.63	13 (38%)
4	FAD	C	1031	-	52,58,58	2.17	21 (40%)	52,89,89	2.01	11 (21%)
2	SF4	D	1026	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	1027	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	1028	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	1029	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	D	1030	-	32,33,33	2.65	10 (31%)	34,50,50	3.65	12 (35%)
4	FAD	D	1031	-	52,58,58	2.13	19 (36%)	52,89,89	2.02	11 (21%)

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	SF4	A	1026	1	-	0/0/48/48	2/6/5/5
2	SF4	A	1027	1	-	0/0/48/48	2/6/5/5
2	SF4	A	1028	1	-	0/0/48/48	2/6/5/5
2	SF4	A	1029	1	-	0/0/48/48	2/6/5/5
3	FMN	A	1030	-	-	0/18/18/18	0/3/3/3
4	FAD	A	1031	-	-	0/30/50/50	0/6/6/6
2	SF4	B	1026	1	-	0/0/48/48	2/6/5/5
2	SF4	B	1027	1	-	0/0/48/48	2/6/5/5
2	SF4	B	1028	1	-	0/0/48/48	2/6/5/5
2	SF4	B	1029	1	-	0/0/48/48	2/6/5/5
3	FMN	B	1030	-	-	0/18/18/18	0/3/3/3
4	FAD	B	1031	-	-	0/30/50/50	0/6/6/6
2	SF4	C	1026	1	-	0/0/48/48	2/6/5/5
2	SF4	C	1027	1	-	0/0/48/48	2/6/5/5
2	SF4	C	1028	1	-	0/0/48/48	2/6/5/5
2	SF4	C	1029	1	-	0/0/48/48	2/6/5/5
3	FMN	C	1030	-	-	0/18/18/18	0/3/3/3
4	FAD	C	1031	-	-	0/30/50/50	0/6/6/6
2	SF4	D	1026	1	-	0/0/48/48	2/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	D	1027	1	-	0/0/48/48	2/6/5/5
2	SF4	D	1028	1	-	0/0/48/48	2/6/5/5
2	SF4	D	1029	1	-	0/0/48/48	2/6/5/5
3	FMN	D	1030	-	-	0/18/18/18	0/3/3/3
4	FAD	D	1031	-	-	0/30/50/50	0/6/6/6

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1030	FMN	C1'-N10	-9.07	1.38	1.48
3	A	1030	FMN	C1'-N10	-9.01	1.38	1.48
3	D	1030	FMN	C1'-N10	-8.93	1.38	1.48
3	B	1030	FMN	C1'-N10	-8.59	1.39	1.48
4	D	1031	FAD	PA-O2A	-4.62	1.35	1.55
4	C	1031	FAD	PA-O2A	-4.60	1.35	1.55
4	B	1031	FAD	PA-O2A	-4.51	1.36	1.55
4	A	1031	FAD	PA-O2A	-4.45	1.36	1.55
4	D	1031	FAD	P-O2P	-3.80	1.39	1.55
4	A	1031	FAD	P-O2P	-3.69	1.39	1.55
4	B	1031	FAD	P-O2P	-3.67	1.39	1.55
4	C	1031	FAD	P-O2P	-3.65	1.39	1.55
4	A	1031	FAD	C2B-C1B	-2.63	1.49	1.53
4	B	1031	FAD	C2B-C1B	-2.51	1.49	1.53
4	C	1031	FAD	C10-N10	-2.47	1.36	1.39
4	D	1031	FAD	C2B-C1B	-2.46	1.49	1.53
4	A	1031	FAD	C10-N10	-2.45	1.36	1.39
4	D	1031	FAD	C2-N1	-2.32	1.33	1.38
3	D	1030	FMN	C6-C5A	-2.25	1.38	1.41
4	B	1031	FAD	C10-N10	-2.21	1.36	1.39
3	A	1030	FMN	C6-C5A	-2.18	1.38	1.41
4	C	1031	FAD	C2B-C1B	-2.15	1.50	1.53
3	B	1030	FMN	C6-C5A	-2.15	1.38	1.41
4	A	1031	FAD	C2-N1	-2.12	1.33	1.38
4	C	1031	FAD	C2-N1	-2.06	1.33	1.38
4	D	1031	FAD	C10-N10	-2.05	1.36	1.39
4	C	1031	FAD	P-O5'	-2.03	1.50	1.59
4	C	1031	FAD	C5B-C4B	2.01	1.58	1.51
4	A	1031	FAD	C2A-N1A	2.03	1.37	1.33
4	A	1031	FAD	C2A-N3A	2.04	1.35	1.32
4	B	1031	FAD	C5B-C4B	2.07	1.58	1.51
3	D	1030	FMN	C4A-C10	2.07	1.44	1.40
4	B	1031	FAD	C2A-N1A	2.08	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1031	FAD	C5B-C4B	2.10	1.58	1.51
3	B	1030	FMN	C4A-C10	2.12	1.44	1.40
4	A	1031	FAD	O4B-C4B	2.16	1.50	1.45
4	C	1031	FAD	C2A-N1A	2.19	1.38	1.33
4	B	1031	FAD	C4A-N3A	2.21	1.38	1.35
4	D	1031	FAD	O4B-C4B	2.22	1.50	1.45
4	C	1031	FAD	O4B-C4B	2.24	1.50	1.45
4	C	1031	FAD	C2A-N3A	2.25	1.36	1.32
3	A	1030	FMN	C4A-C10	2.26	1.45	1.40
3	C	1030	FMN	C9A-C5A	2.33	1.47	1.42
3	C	1030	FMN	C4A-C10	2.35	1.45	1.40
3	C	1030	FMN	C4-C4A	2.36	1.46	1.41
4	D	1031	FAD	C2A-N3A	2.39	1.36	1.32
4	B	1031	FAD	O4B-C4B	2.44	1.50	1.45
4	C	1031	FAD	C4A-N3A	2.47	1.39	1.35
4	A	1031	FAD	C4A-N3A	2.47	1.39	1.35
4	D	1031	FAD	C4A-N3A	2.48	1.39	1.35
4	A	1031	FAD	C5X-N5	2.49	1.39	1.35
4	B	1031	FAD	C2A-N3A	2.52	1.36	1.32
4	C	1031	FAD	C8-C7	2.54	1.47	1.41
4	D	1031	FAD	O5'-C5'	2.55	1.55	1.44
4	B	1031	FAD	O5'-C5'	2.57	1.55	1.44
4	C	1031	FAD	O5'-C5'	2.59	1.55	1.44
4	A	1031	FAD	C2-N3	2.62	1.43	1.38
4	D	1031	FAD	C5X-N5	2.64	1.39	1.35
4	C	1031	FAD	C5X-N5	2.65	1.39	1.35
3	A	1030	FMN	C4-C4A	2.66	1.46	1.41
4	A	1031	FAD	O5'-C5'	2.66	1.55	1.44
4	B	1031	FAD	C5X-N5	2.66	1.39	1.35
3	B	1030	FMN	C4'-C3'	2.69	1.58	1.53
4	B	1031	FAD	C8-C7	2.69	1.48	1.41
3	D	1030	FMN	C4-C4A	2.69	1.46	1.41
4	D	1031	FAD	C8-C7	2.69	1.48	1.41
4	A	1031	FAD	C8-C7	2.71	1.48	1.41
4	C	1031	FAD	C2-N3	2.72	1.43	1.38
4	B	1031	FAD	C2-N3	2.74	1.43	1.38
4	D	1031	FAD	C2-N3	2.78	1.44	1.38
3	D	1030	FMN	C4'-C3'	2.79	1.59	1.53
4	A	1031	FAD	C4-C4X	2.80	1.46	1.41
4	D	1031	FAD	C4-C4X	2.80	1.47	1.41
3	B	1030	FMN	C4-C4A	2.81	1.47	1.41
3	A	1030	FMN	C4'-C3'	2.88	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1030	FMN	C5A-N5	2.88	1.39	1.35
4	B	1031	FAD	C4-C4X	2.98	1.47	1.41
3	C	1030	FMN	C4'-C3'	3.02	1.59	1.53
4	C	1031	FAD	C4-C4X	3.04	1.47	1.41
3	A	1030	FMN	C5A-N5	3.05	1.40	1.35
4	B	1031	FAD	C4X-N5	3.07	1.38	1.33
4	D	1031	FAD	C4X-N5	3.10	1.38	1.33
4	A	1031	FAD	C4X-N5	3.14	1.38	1.33
3	D	1030	FMN	C5A-N5	3.19	1.40	1.35
4	C	1031	FAD	C4X-N5	3.27	1.38	1.33
3	C	1030	FMN	C5A-N5	3.46	1.40	1.35
4	D	1031	FAD	O4B-C1B	3.70	1.46	1.41
4	A	1031	FAD	O4B-C1B	3.78	1.46	1.41
4	A	1031	FAD	C4-N3	3.98	1.40	1.33
4	B	1031	FAD	C4-N3	4.06	1.40	1.33
4	D	1031	FAD	C4-N3	4.07	1.40	1.33
3	D	1030	FMN	C7M-C7	4.07	1.59	1.51
4	C	1031	FAD	C4-N3	4.15	1.40	1.33
4	B	1031	FAD	O4B-C1B	4.16	1.47	1.41
4	A	1031	FAD	C4X-C10	4.17	1.48	1.40
4	C	1031	FAD	O4B-C1B	4.19	1.47	1.41
3	C	1030	FMN	C4-N3	4.20	1.40	1.33
3	C	1030	FMN	C7M-C7	4.24	1.59	1.51
3	D	1030	FMN	C4-N3	4.24	1.40	1.33
4	C	1031	FAD	C4X-C10	4.25	1.48	1.40
3	A	1030	FMN	C4-N3	4.26	1.40	1.33
3	B	1030	FMN	C4A-N5	4.28	1.39	1.33
3	B	1030	FMN	C4-N3	4.29	1.40	1.33
3	B	1030	FMN	C7M-C7	4.31	1.59	1.51
4	D	1031	FAD	C4X-C10	4.34	1.48	1.40
3	A	1030	FMN	C7M-C7	4.36	1.59	1.51
4	B	1031	FAD	C4X-C10	4.42	1.49	1.40
3	A	1030	FMN	C4A-N5	4.69	1.40	1.33
3	C	1030	FMN	C4A-N5	4.72	1.40	1.33
3	D	1030	FMN	C4A-N5	4.76	1.40	1.33
3	B	1030	FMN	C9A-N10	4.83	1.45	1.38
3	D	1030	FMN	C9A-N10	5.06	1.46	1.38
3	A	1030	FMN	C9A-N10	5.20	1.46	1.38
3	C	1030	FMN	C9A-N10	5.39	1.46	1.38
4	D	1031	FAD	C9A-N10	5.52	1.46	1.38
4	A	1031	FAD	C9A-N10	5.84	1.47	1.38
4	C	1031	FAD	C9A-N10	5.91	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1031	FAD	C9A-N10	5.98	1.47	1.38

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1030	FMN	C4A-C4-N3	-8.51	112.40	123.52
3	A	1030	FMN	C4A-C4-N3	-8.48	112.43	123.52
3	B	1030	FMN	C4A-C4-N3	-8.40	112.54	123.52
3	C	1030	FMN	C4A-C4-N3	-8.38	112.57	123.52
3	B	1030	FMN	N3-C2-N1	-7.51	115.05	127.69
3	D	1030	FMN	N3-C2-N1	-7.49	115.07	127.69
3	A	1030	FMN	N3-C2-N1	-7.39	115.25	127.69
3	C	1030	FMN	N3-C2-N1	-7.37	115.28	127.69
4	D	1031	FAD	C4X-C4-N3	-4.93	117.08	123.52
4	C	1031	FAD	C4X-C4-N3	-4.80	117.25	123.52
4	B	1031	FAD	C4X-C4-N3	-4.66	117.44	123.52
4	A	1031	FAD	C4X-C4-N3	-4.64	117.45	123.52
4	C	1031	FAD	C4-C4X-C10	-4.16	117.28	119.94
4	D	1031	FAD	N3A-C2A-N1A	-4.06	125.68	128.87
4	B	1031	FAD	C4-C4X-C10	-4.02	117.37	119.94
4	A	1031	FAD	C4-C4X-C10	-4.01	117.38	119.94
4	C	1031	FAD	O2A-PA-O3P	-3.98	88.22	105.27
4	D	1031	FAD	C4-C4X-C10	-3.95	117.41	119.94
4	B	1031	FAD	O2A-PA-O3P	-3.95	88.33	105.27
4	A	1031	FAD	N3A-C2A-N1A	-3.88	125.83	128.87
4	A	1031	FAD	O2A-PA-O3P	-3.86	88.74	105.27
4	D	1031	FAD	O2A-PA-O3P	-3.80	88.98	105.27
4	C	1031	FAD	N3-C2-N1	-3.74	121.40	127.69
4	D	1031	FAD	N3-C2-N1	-3.71	121.44	127.69
4	B	1031	FAD	N3A-C2A-N1A	-3.71	125.96	128.87
4	A	1031	FAD	N3-C2-N1	-3.68	121.49	127.69
4	B	1031	FAD	N3-C2-N1	-3.65	121.55	127.69
4	C	1031	FAD	N3A-C2A-N1A	-3.60	126.04	128.87
3	D	1030	FMN	O3'-C3'-C2'	-3.40	99.91	108.73
3	A	1030	FMN	O3'-C3'-C2'	-3.39	99.94	108.73
3	B	1030	FMN	O3'-C3'-C2'	-3.27	100.26	108.73
3	C	1030	FMN	O3'-C3'-C2'	-3.13	100.62	108.73
3	C	1030	FMN	C4-C4A-N5	-2.96	115.10	118.70
4	A	1031	FAD	O4B-C1B-N9A	-2.89	102.64	108.11
4	B	1031	FAD	O4B-C1B-N9A	-2.89	102.65	108.11
4	C	1031	FAD	O4B-C1B-N9A	-2.88	102.67	108.11
4	D	1031	FAD	O4B-C1B-N9A	-2.87	102.67	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1030	FMN	C4-C4A-N5	-2.81	115.27	118.70
3	D	1030	FMN	C4-C4A-N5	-2.74	115.36	118.70
3	A	1030	FMN	C4-C4A-N5	-2.62	115.51	118.70
4	A	1031	FAD	C5X-C9A-N10	-2.31	115.85	117.58
4	C	1031	FAD	C4X-C10-N10	-2.27	118.87	120.52
4	B	1031	FAD	C4X-C10-N10	-2.23	118.90	120.52
4	B	1031	FAD	C5X-C9A-N10	-2.12	115.99	117.58
3	B	1030	FMN	C7-C6-C5A	-2.11	117.45	120.90
4	C	1031	FAD	C5X-C9A-N10	-2.11	116.00	117.58
4	D	1031	FAD	C5X-C9A-N10	-2.11	116.00	117.58
3	C	1030	FMN	C7-C6-C5A	-2.10	117.47	120.90
4	A	1031	FAD	C4X-C10-N10	-2.08	119.01	120.52
4	D	1031	FAD	C4X-C10-N10	-2.07	119.02	120.52
3	C	1030	FMN	O3'-C3'-C4'	2.12	114.23	108.73
3	A	1030	FMN	O3'-C3'-C4'	2.19	114.40	108.73
4	C	1031	FAD	C2A-N1A-C6A	2.21	122.71	118.77
3	D	1030	FMN	O3'-C3'-C4'	2.21	114.45	108.73
4	D	1031	FAD	C2A-N1A-C6A	2.25	122.79	118.77
4	B	1031	FAD	C2A-N1A-C6A	2.30	122.87	118.77
3	D	1030	FMN	C6-C5A-C9A	2.38	121.73	119.11
3	B	1030	FMN	O3'-C3'-C4'	2.39	114.92	108.73
4	A	1031	FAD	C2A-N1A-C6A	2.42	123.09	118.77
3	A	1030	FMN	C6-C5A-C9A	2.58	121.95	119.11
3	B	1030	FMN	C6-C5A-C9A	2.61	121.98	119.11
3	C	1030	FMN	C6-C5A-C9A	2.63	122.01	119.11
3	C	1030	FMN	C4A-N5-C5A	2.67	119.87	116.72
3	D	1030	FMN	C4A-N5-C5A	2.80	120.02	116.72
3	A	1030	FMN	C4A-N5-C5A	2.81	120.03	116.72
3	B	1030	FMN	C4A-N5-C5A	2.89	120.12	116.72
4	C	1031	FAD	O2A-PA-O1A	3.14	128.89	112.56
3	B	1030	FMN	C1'-N10-C9A	3.23	122.57	118.83
3	D	1030	FMN	C1'-N10-C9A	3.24	122.58	118.83
3	A	1030	FMN	C1'-N10-C9A	3.27	122.62	118.83
4	B	1031	FAD	O2A-PA-O1A	3.28	129.62	112.56
4	A	1031	FAD	O2A-PA-O1A	3.30	129.75	112.56
3	C	1030	FMN	O2'-C2'-C1'	3.34	118.19	109.93
4	D	1031	FAD	O2A-PA-O1A	3.35	129.99	112.56
3	B	1030	FMN	O2'-C2'-C1'	3.38	118.27	109.93
3	A	1030	FMN	O2'-C2'-C1'	3.38	118.28	109.93
3	D	1030	FMN	O2'-C2'-C1'	3.39	118.31	109.93
3	C	1030	FMN	C1'-N10-C9A	3.47	122.85	118.83
3	B	1030	FMN	O4'-C4'-C3'	3.56	118.13	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1030	FMN	O4'-C4'-C3'	3.59	118.20	108.96
3	A	1030	FMN	O4'-C4'-C3'	3.69	118.44	108.96
3	C	1030	FMN	O4'-C4'-C3'	3.73	118.56	108.96
3	A	1030	FMN	C4-C4A-C10	5.77	123.63	119.94
3	D	1030	FMN	C4-C4A-C10	5.78	123.64	119.94
3	C	1030	FMN	C4-C4A-C10	5.86	123.69	119.94
3	B	1030	FMN	C4-C4A-C10	5.91	123.72	119.94
4	A	1031	FAD	C4-N3-C2	7.84	121.70	115.16
4	B	1031	FAD	C4-N3-C2	7.98	121.81	115.16
4	C	1031	FAD	C4-N3-C2	8.05	121.87	115.16
4	D	1031	FAD	C4-N3-C2	8.12	121.94	115.16
3	B	1030	FMN	C4-N3-C2	13.80	126.67	115.16
3	C	1030	FMN	C4-N3-C2	13.85	126.71	115.16
3	A	1030	FMN	C4-N3-C2	14.02	126.86	115.16
3	D	1030	FMN	C4-N3-C2	14.12	126.94	115.16

There are no chirality outliers.

There are no torsion outliers.

All (32) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1029	SF4	FE1-FE2-S3-S4
2	B	1027	SF4	FE3-FE4-S1-S2
2	C	1029	SF4	FE1-FE2-S3-S4
2	B	1029	SF4	FE1-FE2-S3-S4
2	A	1029	SF4	FE1-FE2-S3-S4
2	A	1027	SF4	FE3-FE4-S1-S2
2	A	1026	SF4	FE1-FE2-S3-S4
2	D	1027	SF4	FE3-FE4-S1-S2
2	B	1026	SF4	FE3-FE4-S1-S2
2	C	1027	SF4	FE3-FE4-S1-S2
2	C	1028	SF4	FE1-FE2-S3-S4
2	C	1026	SF4	FE3-FE4-S1-S2
2	A	1028	SF4	FE3-FE4-S1-S2
2	D	1028	SF4	FE1-FE2-S3-S4
2	D	1027	SF4	FE1-FE2-S3-S4
2	D	1026	SF4	FE3-FE4-S1-S2
2	D	1026	SF4	FE1-FE2-S3-S4
2	B	1028	SF4	FE1-FE2-S3-S4
2	A	1028	SF4	FE1-FE2-S3-S4
2	B	1026	SF4	FE1-FE2-S3-S4

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Mol	Chain	Res	Type	Atoms
2	A	1026	SF4	FE3-FE4-S1-S2
2	C	1027	SF4	FE1-FE2-S3-S4
2	A	1027	SF4	FE1-FE2-S3-S4
2	B	1028	SF4	FE3-FE4-S1-S2
2	C	1026	SF4	FE1-FE2-S3-S4
2	C	1028	SF4	FE3-FE4-S1-S2
2	D	1028	SF4	FE3-FE4-S1-S2
2	B	1029	SF4	FE3-FE4-S1-S2
2	C	1029	SF4	FE3-FE4-S1-S2
2	B	1027	SF4	FE1-FE2-S3-S4
2	A	1029	SF4	FE3-FE4-S1-S2
2	D	1029	SF4	FE3-FE4-S1-S2

12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1027	SF4	1	0
3	A	1030	FMN	1	0
4	A	1031	FAD	2	0
2	B	1026	SF4	1	0
2	B	1027	SF4	1	0
3	B	1030	FMN	1	0
4	B	1031	FAD	2	0
2	C	1026	SF4	1	0
4	C	1031	FAD	2	0
2	D	1026	SF4	1	0
2	D	1027	SF4	1	0
4	D	1031	FAD	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1007/1025 (98%)	0.21	68 (6%)	20	23	7, 14, 36, 56	0
1	B	1007/1025 (98%)	0.23	77 (7%)	17	18	6, 14, 36, 55	0
1	C	1012/1025 (98%)	0.22	73 (7%)	18	20	6, 14, 38, 54	0
1	D	1012/1025 (98%)	0.24	82 (8%)	15	16	6, 14, 37, 55	0
All	All	4038/4100 (98%)	0.22	300 (7%)	17	19	6, 14, 37, 56	0

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	18.1
1	A	1017	LEU	16.1
1	D	2	ALA	16.0
1	C	1017	LEU	14.9
1	A	2	ALA	14.4
1	C	2	ALA	12.6
1	B	907	LEU	12.3
1	D	907	LEU	12.0
1	A	907	LEU	11.6
1	D	52	CYS	11.2
1	D	1017	LEU	10.0
1	B	1017	LEU	9.2
1	B	1018	PRO	9.0
1	A	324	CYS	8.9
1	C	674	GLY	8.8
1	C	675	MET	8.7
1	B	51	HIS	8.4
1	D	902	ALA	7.8
1	C	415	GLU	7.6
1	A	51	HIS	7.4
1	B	52	CYS	7.4

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Mol	Chain	Res	Type	RSRZ
1	B	680	MET	7.2
1	A	867	ARG	7.1
1	D	50	PHE	7.1
1	C	51	HIS	7.0
1	A	325	HIS	6.9
1	D	51	HIS	6.8
1	D	459	TRP	6.8
1	A	416	THR	6.8
1	D	901	ASN	6.6
1	B	415	GLU	6.6
1	B	872	MET	6.6
1	A	52	CYS	6.6
1	B	416	THR	6.5
1	C	417	GLY	6.5
1	A	675	MET	6.4
1	B	908	GLU	6.3
1	D	867	ARG	6.2
1	A	908	GLU	6.2
1	C	872	MET	6.1
1	A	175	CYS	6.1
1	C	680	MET	6.0
1	B	902	ALA	6.0
1	A	417	GLY	6.0
1	A	902	ALA	6.0
1	D	415	GLU	5.9
1	B	900	GLN	5.8
1	C	867	ARG	5.8
1	B	459	TRP	5.8
1	C	682	LEU	5.7
1	B	323	ALA	5.7
1	D	175	CYS	5.6
1	B	867	ARG	5.6
1	B	417	GLY	5.6
1	A	418	LYS	5.6
1	A	415	GLU	5.5
1	C	50	PHE	5.5
1	C	416	THR	5.5
1	C	410	ARG	5.4
1	D	872	MET	5.3
1	A	1016	GLY	5.2
1	C	53	GLU	5.2
1	D	679	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	417	GLY	5.2
1	D	1018	PRO	5.2
1	D	53	GLU	5.2
1	D	909	ARG	5.2
1	D	899	GLU	5.1
1	B	175	CYS	5.1
1	C	681	GLY	5.1
1	A	682	LEU	5.1
1	D	418	LYS	5.0
1	A	1010	PRO	5.0
1	B	682	LEU	5.0
1	A	458	ARG	5.0
1	C	459	TRP	4.9
1	B	673	HIS	4.8
1	C	332	ARG	4.8
1	C	175	CYS	4.8
1	D	1010	PRO	4.7
1	B	901	ASN	4.7
1	D	674	GLY	4.6
1	C	325	HIS	4.6
1	A	322	CYS	4.6
1	A	681	GLY	4.6
1	D	866	PRO	4.5
1	C	52	CYS	4.5
1	A	1009	THR	4.5
1	D	414	ASP	4.4
1	C	673	HIS	4.4
1	D	458	ARG	4.4
1	A	673	HIS	4.3
1	B	1010	PRO	4.3
1	B	180	GLU	4.2
1	B	424	ASP	4.2
1	D	3	PRO	4.2
1	B	325	HIS	4.1
1	B	418	LYS	4.1
1	B	1011	TYR	4.1
1	C	899	GLU	4.1
1	B	869	ALA	4.1
1	C	909	ARG	4.0
1	B	324	CYS	4.0
1	D	856	THR	4.0
1	A	901	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	326	SER	4.0
1	B	322	CYS	3.9
1	B	458	ARG	3.9
1	D	908	GLU	3.9
1	B	410	ARG	3.8
1	C	873	GLY	3.8
1	D	54	LYS	3.8
1	C	517	ALA	3.8
1	D	1009	THR	3.8
1	C	324	CYS	3.7
1	C	908	GLU	3.7
1	D	416	THR	3.7
1	A	900	GLN	3.6
1	D	678	ARG	3.6
1	B	367	PHE	3.6
1	D	680	MET	3.6
1	A	179	GLN	3.5
1	C	330	SER	3.5
1	C	414	ASP	3.5
1	D	1019	LEU	3.5
1	D	410	ARG	3.5
1	B	3	PRO	3.5
1	B	53	GLU	3.5
1	D	900	GLN	3.5
1	A	872	MET	3.5
1	D	868	ILE	3.4
1	D	913	ILE	3.4
1	B	443	ARG	3.4
1	C	900	GLN	3.4
1	A	49	CYS	3.4
1	C	423	GLU	3.4
1	A	517	ALA	3.4
1	D	1012	GLU	3.4
1	C	870	GLU	3.4
1	A	459	TRP	3.3
1	D	296	GLY	3.3
1	A	414	ASP	3.3
1	B	520	GLU	3.3
1	C	458	ARG	3.3
1	B	421	GLU	3.3
1	C	323	ALA	3.3
1	C	180	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	295	GLN	3.3
1	B	49	CYS	3.3
1	D	855	GLY	3.2
1	D	367	PHE	3.2
1	A	870	GLU	3.2
1	B	50	PHE	3.2
1	D	1011	TYR	3.2
1	C	402	ARG	3.2
1	D	179	GLN	3.1
1	A	180	GLU	3.1
1	B	519	PRO	3.1
1	C	869	ALA	3.1
1	D	870	GLU	3.1
1	C	367	PHE	3.1
1	D	675	MET	3.1
1	B	326	SER	3.1
1	D	869	ALA	3.1
1	C	487	ASN	3.0
1	D	420	ASN	3.0
1	B	899	GLU	3.0
1	C	910	LYS	3.0
1	C	847	GLN	3.0
1	D	517	ALA	3.0
1	A	3	PRO	3.0
1	D	857	GLU	3.0
1	A	896	ARG	3.0
1	B	517	ALA	3.0
1	A	367	PHE	2.9
1	A	518	LYS	2.9
1	D	180	GLU	2.9
1	A	1012	GLU	2.8
1	C	424	ASP	2.8
1	A	273	GLU	2.8
1	D	917	PRO	2.8
1	D	423	GLU	2.8
1	D	264	ASN	2.8
1	B	847	GLN	2.8
1	C	49	CYS	2.8
1	A	319	ALA	2.7
1	A	11	ASP	2.7
1	B	179	GLN	2.7
1	B	413	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	426	ILE	2.7
1	C	904	PHE	2.7
1	A	674	GLY	2.7
1	D	36	LEU	2.7
1	B	518	LYS	2.7
1	D	1014	LYS	2.7
1	A	36	LEU	2.7
1	D	11	ASP	2.7
1	D	291	ASP	2.6
1	B	427	VAL	2.6
1	D	443	ARG	2.6
1	B	273	GLU	2.6
1	D	682	LEU	2.6
1	C	327	PRO	2.6
1	D	896	ARG	2.6
1	B	681	GLY	2.6
1	C	264	ASN	2.6
1	D	173	ASN	2.6
1	B	414	ASP	2.6
1	B	36	LEU	2.5
1	C	36	LEU	2.5
1	C	371	ARG	2.5
1	C	419	TRP	2.5
1	A	292	ASP	2.5
1	B	896	ARG	2.5
1	D	371	ARG	2.5
1	A	917	PRO	2.5
1	C	418	LYS	2.5
1	D	364	ARG	2.5
1	A	23	GLN	2.5
1	C	407	GLN	2.5
1	C	1010	PRO	2.5
1	A	910	LYS	2.5
1	A	426	ILE	2.5
1	D	915	LYS	2.5
1	C	273	GLU	2.5
1	B	423	GLU	2.5
1	D	859	HIS	2.5
1	A	1011	TYR	2.5
1	B	375	GLU	2.5
1	A	868	ILE	2.4
1	B	941	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	599	MET	2.4
1	D	273	GLU	2.4
1	A	696	ARG	2.4
1	D	49	CYS	2.4
1	C	518	LYS	2.4
1	C	874	LYS	2.4
1	C	331	ILE	2.4
1	D	427	VAL	2.4
1	A	50	PHE	2.4
1	A	181	LYS	2.4
1	C	516	SER	2.3
1	D	910	LYS	2.3
1	D	1008	THR	2.3
1	D	487	ASN	2.3
1	C	3	PRO	2.3
1	A	424	ASP	2.3
1	D	395	LYS	2.3
1	B	859	HIS	2.3
1	D	322	CYS	2.3
1	A	869	ALA	2.3
1	C	903	ALA	2.3
1	B	22	THR	2.3
1	A	402	ARG	2.3
1	D	865	VAL	2.3
1	B	485	MET	2.3
1	B	332	ARG	2.3
1	B	371	ARG	2.3
1	A	410	ARG	2.3
1	C	11	ASP	2.3
1	B	173	ASN	2.3
1	C	7	LYS	2.3
1	A	323	ALA	2.2
1	B	11	ASP	2.2
1	B	221	GLU	2.2
1	A	371	ARG	2.2
1	B	873	GLY	2.2
1	B	402	ARG	2.2
1	C	984	ASP	2.2
1	C	1009	THR	2.2
1	A	844	GLU	2.2
1	C	896	ARG	2.2
1	B	395	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	844	GLU	2.2
1	C	179	GLN	2.2
1	B	1012	GLU	2.2
1	B	54	LYS	2.2
1	B	181	LYS	2.2
1	A	857	GLU	2.1
1	C	443	ARG	2.1
1	D	402	ARG	2.1
1	D	874	LYS	2.1
1	A	393	PRO	2.1
1	A	22	THR	2.1
1	D	323	ALA	2.1
1	A	899	GLU	2.1
1	B	910	LYS	2.1
1	A	941	ILE	2.1
1	B	420	ASN	2.1
1	A	885	GLN	2.1
1	B	327	PRO	2.1
1	A	375	GLU	2.1
1	C	184	GLU	2.1
1	C	1012	GLU	2.1
1	D	176	LEU	2.1
1	D	325	HIS	2.0
1	B	320	GLY	2.0
1	B	396	VAL	2.0
1	B	295	GLN	2.0
1	C	420	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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
2	SF4	A	1027	8/8	0.97	0.10	0.63	8,9,11,12	0
2	SF4	B	1026	8/8	0.97	0.10	0.51	10,10,12,12	0
2	SF4	C	1027	8/8	0.97	0.10	0.42	8,9,11,11	0
3	FMN	A	1030	31/31	0.96	0.09	0.11	8,10,13,13	0
4	FAD	B	1031	53/53	0.97	0.10	0.10	9,12,14,15	0
2	SF4	A	1028	8/8	0.97	0.09	0.00	9,11,11,13	0
4	FAD	A	1031	53/53	0.96	0.10	-0.04	8,11,13,14	0
2	SF4	B	1029	8/8	0.97	0.09	-0.10	10,11,13,13	0
2	SF4	D	1028	8/8	0.97	0.09	-0.11	9,10,12,12	0
2	SF4	C	1026	8/8	0.97	0.09	-0.13	10,10,12,12	0
2	SF4	A	1026	8/8	0.97	0.09	-0.17	10,10,12,12	0
3	FMN	B	1030	31/31	0.97	0.09	-0.18	7,10,12,15	0
2	SF4	C	1029	8/8	0.97	0.09	-0.19	9,10,12,12	0
3	FMN	D	1030	31/31	0.97	0.08	-0.20	7,10,12,13	0
2	SF4	B	1028	8/8	0.97	0.09	-0.23	10,11,12,13	0
2	SF4	D	1027	8/8	0.97	0.09	-0.28	7,8,10,11	0
2	SF4	D	1029	8/8	0.97	0.09	-0.38	10,11,12,13	0
4	FAD	D	1031	53/53	0.97	0.09	-0.42	8,11,13,14	0
3	FMN	C	1030	31/31	0.97	0.09	-0.44	8,9,12,15	0
2	SF4	D	1026	8/8	0.97	0.09	-0.49	9,10,11,12	0
2	SF4	A	1029	8/8	0.97	0.09	-0.55	10,11,13,13	0
2	SF4	B	1027	8/8	0.97	0.09	-0.61	8,9,11,11	0
4	FAD	C	1031	53/53	0.97	0.08	-0.64	7,11,14,15	0
2	SF4	C	1028	8/8	0.97	0.09	-0.82	8,9,10,12	0

6.5 Other polymers (i)

There are no such residues in this entry.