



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2018 – 09:21 AM EST

PDB ID : 1GTE
Title : DIHYDROPYRIMIDINE DEHYDROGENASE (DPD) FROM PIG, BINARY
COMPLEX WITH 5-IOLOURACIL
Authors : Dobritsch, D.; Ricagno, S.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on : 2002-01-15
Resolution : 1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

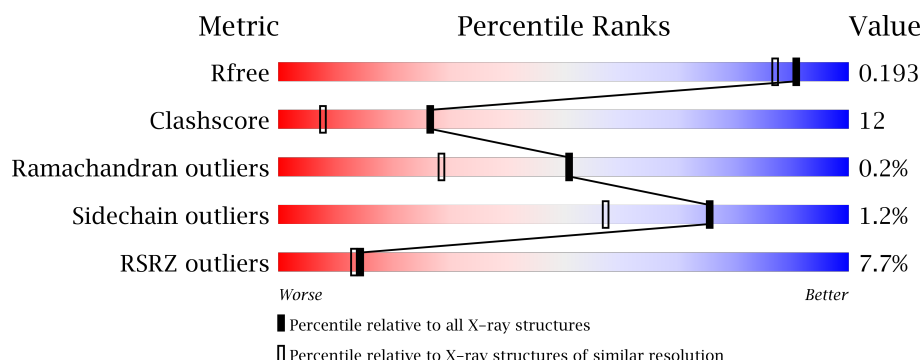
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1368 (1.66-1.66)
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)
RSRZ outliers	101464	1371 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1025	
1	B	1025	
1	C	1025	
1	D	1025	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36226 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	1005	Total	C	N	O	S	0	4	0
			7683	4872	1300	1456	55			
1	B	1005	Total	C	N	O	S	0	5	0
			7693	4877	1304	1457	55			
1	C	1010	Total	C	N	O	S	0	11	0
			7748	4920	1309	1464	55			
1	D	1014	Total	C	N	O	S	0	7	0
			7754	4916	1312	1470	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: Fe₄S₄).



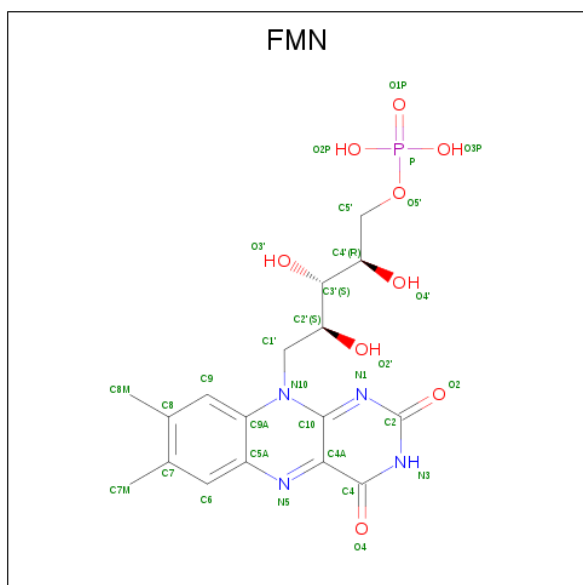
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2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

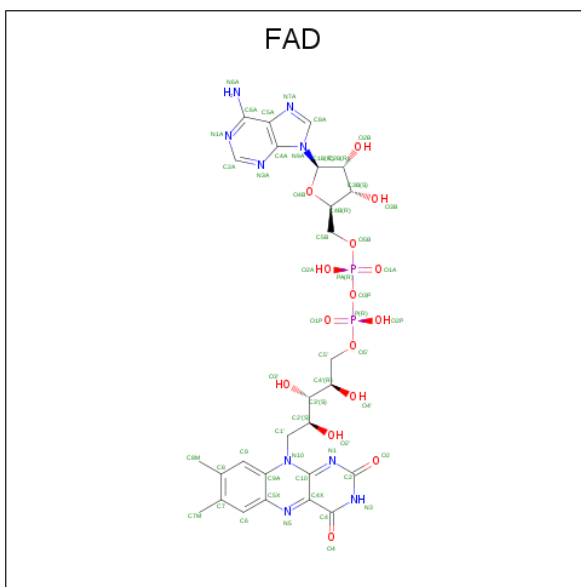
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

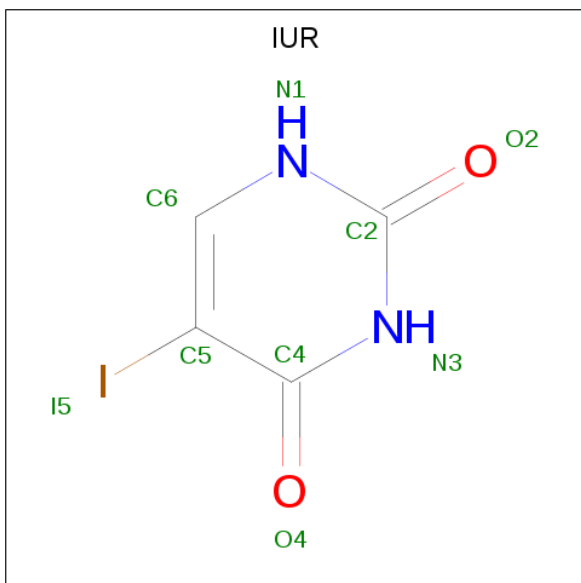
- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).





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

- Molecule 5 is 5-iodouracil (three-letter code: IUR) (formula: $C_4H_3IN_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	I	N	O	
			9	4	1	2	2	
5	B	1	Total	C	I	N	O	
			9	4	1	2	2	
5	C	1	Total	C	I	N	O	
			9	4	1	2	2	
5	D	1	Total	C	I	N	O	
			9	4	1	2	2	

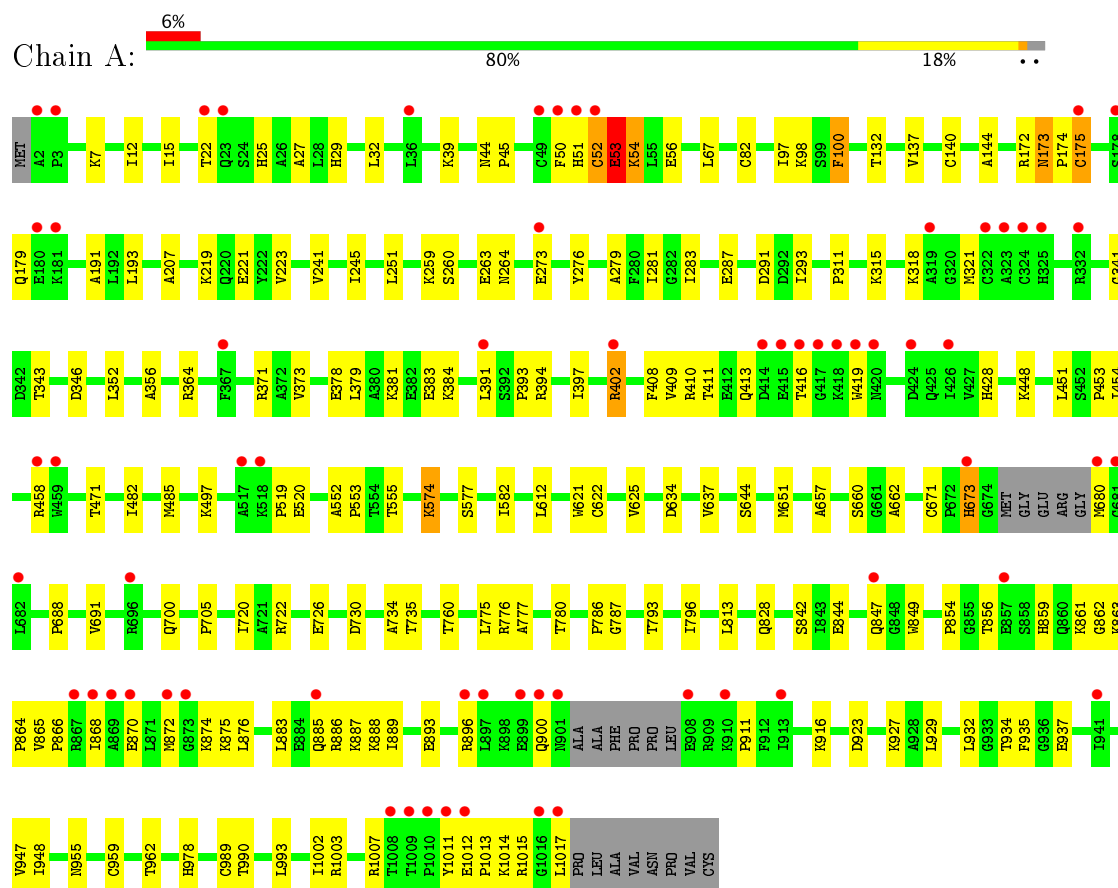
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1170	Total	O		
			1170	1170	0	0
6	B	1221	Total	O		
			1221	1221	0	0
6	C	1189	Total	O		
			1189	1189	0	0
6	D	1268	Total	O		
			1268	1268	0	0

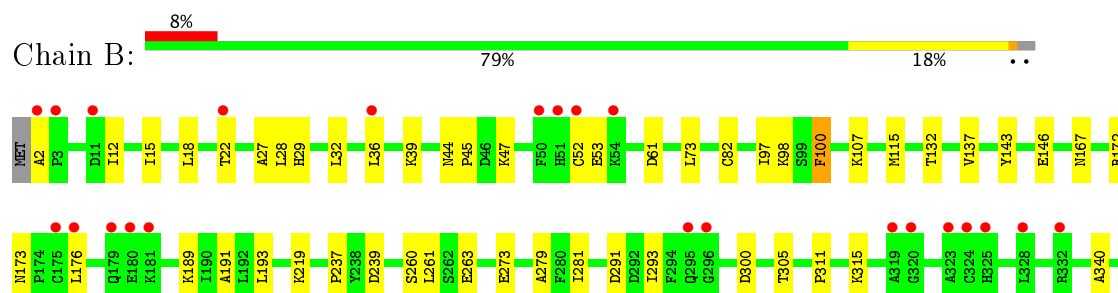
3 Residue-property plots

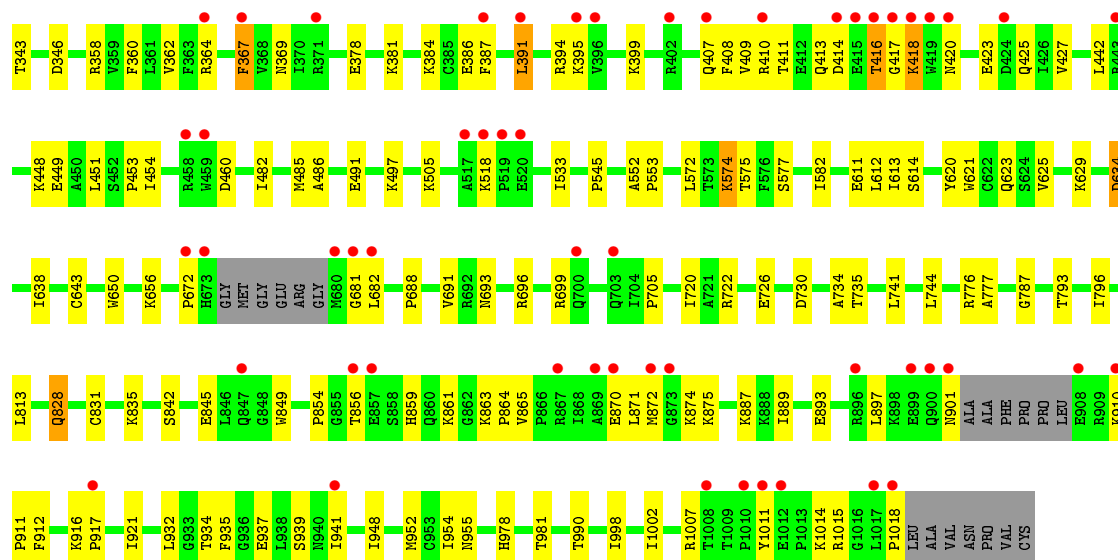
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

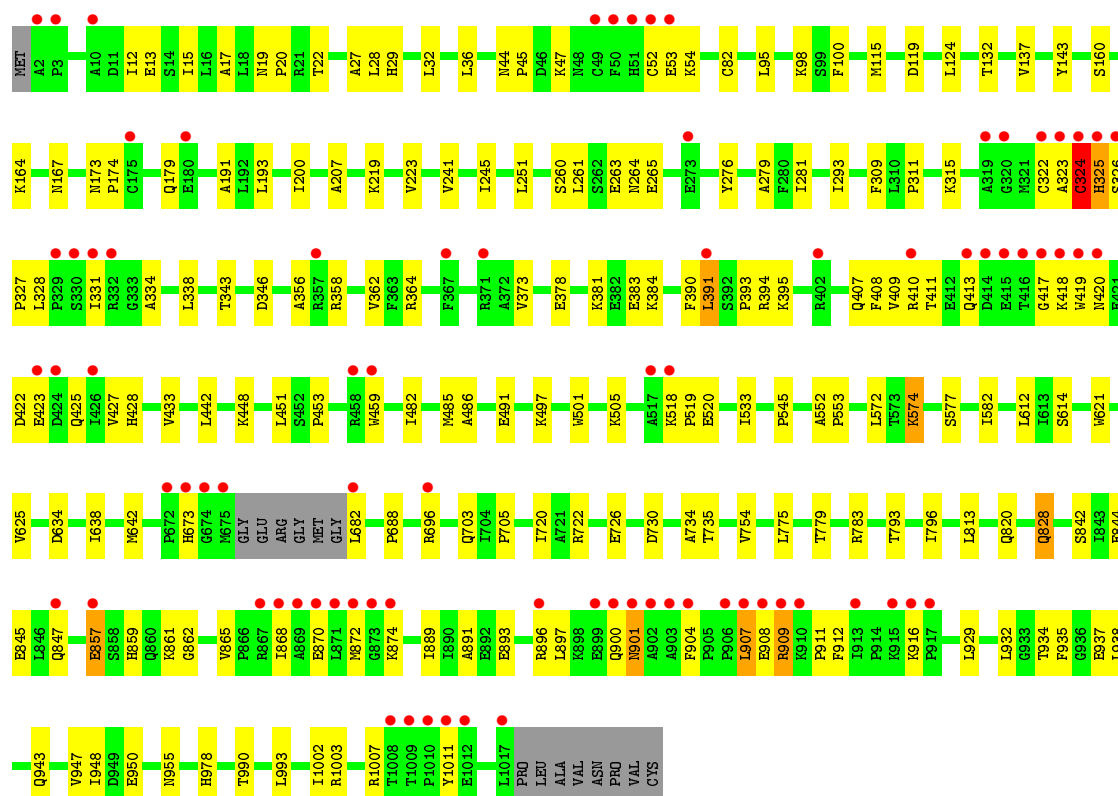
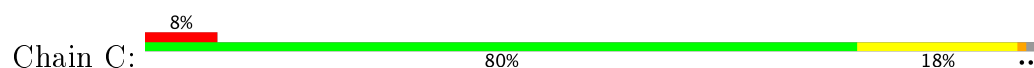


• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

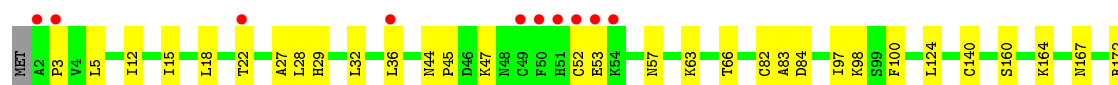
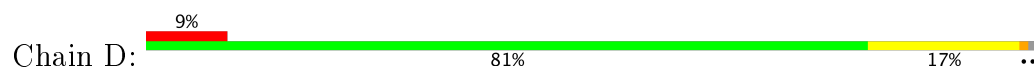


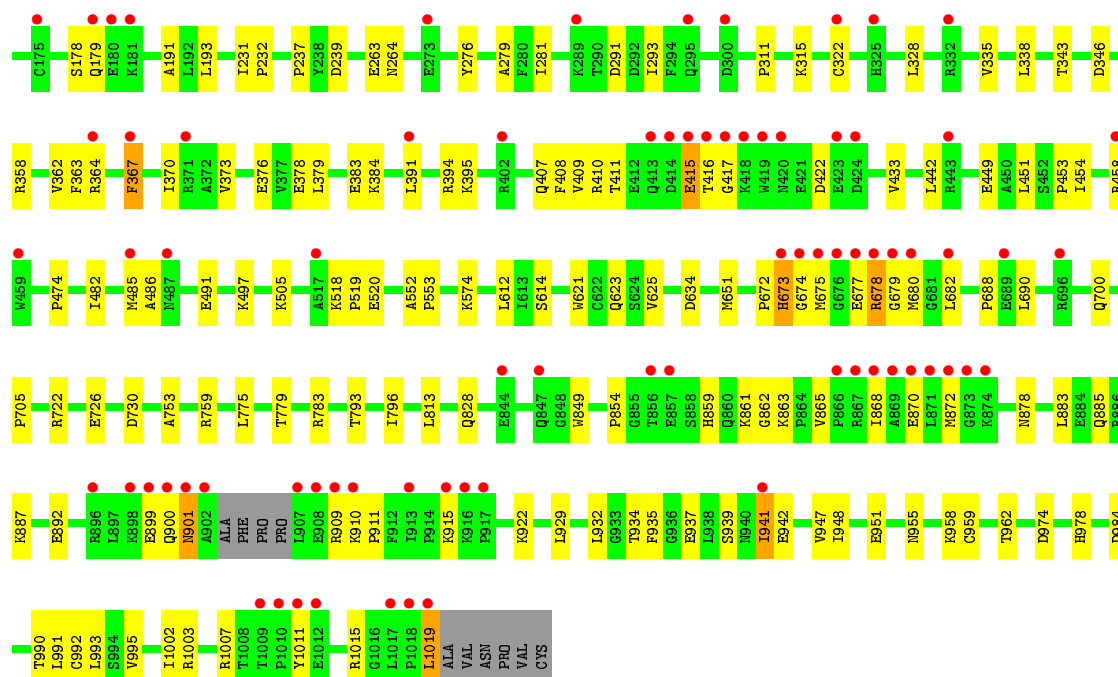


• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE



• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.71Å 158.37Å 162.33Å 90.00° 95.84° 90.00°	Depositor
Resolution (Å)	24.98 – 1.65 24.98 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.0 (24.98-1.65) 98.1 (24.98-1.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 1.65Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.181 , 0.197 0.178 , 0.193	Depositor DCC
R_{free} test set	9508 reflections (2.01%)	DCC
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36226	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, IUR, 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	0.30	0/7855	0.59	0/10643
1	B	0.30	0/7870	0.59	2/10663 (0.0%)
1	C	0.31	0/7952	0.59	0/10779
1	D	0.30	0/7940	0.58	0/10759
All	All	0.30	0/31617	0.59	2/42844 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	634	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	B	305	THR	N-CA-C	-5.03	97.42	111.00

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	7683	0	7711	173	0
1	B	7693	0	7719	206	0
1	C	7748	0	7785	194	0
1	D	7754	0	7785	189	0
2	A	32	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	32	0	0	1	0
2	C	32	0	0	0	0
2	D	32	0	0	2	0
3	A	31	0	19	1	0
3	B	31	0	19	0	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	9	0	3	1	0
5	B	9	0	3	1	0
5	C	9	0	3	0	0
5	D	9	0	3	0	0
6	A	1170	0	0	60	1
6	B	1221	0	0	80	0
6	C	1189	0	0	50	0
6	D	1268	0	0	63	0
All	All	36226	0	31212	729	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 12.

All (729) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:835:LYS:HG3	6:B:3001:HOH:O	1.45	1.14
1:B:391:LEU:HD23	1:B:410[B]:ARG:HH22	1.10	1.12
1:D:673:HIS:CD2	1:D:675:MET:H	1.68	1.11
1:C:754:VAL:HG23	6:C:2919:HOH:O	1.53	1.06
1:D:779[B]:THR:HG21	1:D:932:LEU:HD22	1.38	1.05
1:B:413:GLN:HG2	1:B:417:GLY:O	1.56	1.05
1:A:352:LEU:HA	6:A:2542:HOH:O	1.62	0.99
1:B:634:ASP:OD1	6:B:2852:HOH:O	1.81	0.98
1:B:613:ILE:HA	6:B:3212:HOH:O	1.64	0.97
1:C:779[B]:THR:HG21	1:C:932[B]:LEU:HD22	1.44	0.97
1:D:673:HIS:HD2	1:D:675:MET:H	0.98	0.97
1:A:657:ALA:HA	6:A:2851:HOH:O	1.65	0.94
1:B:575:THR:HB	6:B:3212:HOH:O	1.68	0.91
1:C:391:LEU:HD23	1:C:410[B]:ARG:HH22	1.33	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167[B]:ASN:HD22	1:B:911:PRO:HA	1.37	0.90
1:A:866:PRO:HD2	6:A:3029:HOH:O	1.72	0.89
1:C:381:LYS:HB3	6:C:2584:HOH:O	1.73	0.88
1:A:321:MET:HA	6:A:2388:HOH:O	1.74	0.85
1:B:408:PHE:HB3	1:B:410[B]:ARG:NH2	1.91	0.85
1:C:322:CYS:SG	1:C:324:CYS:HB3	2.17	0.85
1:B:391:LEU:HD23	1:B:410[B]:ARG:NH2	1.90	0.84
1:B:623:GLN:NE2	6:B:2841:HOH:O	2.11	0.84
1:B:612:LEU:HA	6:B:2825:HOH:O	1.76	0.84
1:C:938:LEU:HA	6:C:3080:HOH:O	1.76	0.83
1:C:634:ASP:OD1	6:C:2816:HOH:O	1.97	0.83
1:A:859:HIS:HD2	1:A:862:GLY:H	1.26	0.83
1:C:324:CYS:SG	1:C:325:HIS:N	2.52	0.82
1:B:533:ILE:HD13	6:B:3001:HOH:O	1.77	0.82
1:B:954:ILE:HG23	1:B:998:ILE:HD11	1.60	0.82
1:B:409:VAL:C	1:B:410[B]:ARG:HE	1.83	0.82
1:C:859:HIS:HD2	1:C:862:GLY:H	1.27	0.81
1:B:381:LYS:HB3	6:B:2627:HOH:O	1.79	0.81
1:B:408:PHE:CB	1:B:410[B]:ARG:NH2	2.43	0.81
1:C:356:ALA:HA	6:C:2520:HOH:O	1.80	0.80
1:B:391:LEU:CD2	1:B:410[B]:ARG:HH12	1.94	0.80
1:B:410[B]:ARG:HD3	1:B:427:VAL:HG23	1.63	0.80
1:D:779[B]:THR:HG21	1:D:932:LEU:CD2	2.11	0.79
1:B:107:LYS:HE3	6:B:2192:HOH:O	1.82	0.79
1:A:929:LEU:HD12	1:D:941:ILE:HG21	1.65	0.79
1:B:73:LEU:HD11	6:B:2192:HOH:O	1.81	0.79
1:B:1014:LYS:HG3	6:B:3202:HOH:O	1.82	0.78
1:C:391:LEU:HD23	1:C:410[B]:ARG:NH2	1.97	0.78
1:D:859:HIS:HD2	1:D:862:GLY:H	1.28	0.78
1:B:394:ARG:HG3	1:B:409:VAL:HG13	1.66	0.78
1:A:844:GLU:O	1:A:847:GLN:HG3	1.84	0.77
1:B:409:VAL:N	1:B:410[B]:ARG:HH21	1.82	0.77
1:C:343:THR:HA	4:C:1031:FAD:HM73	1.66	0.77
1:B:386:GLU:HG2	6:B:2586:HOH:O	1.84	0.77
1:D:673:HIS:HD2	1:D:675:MET:N	1.79	0.77
1:D:394:ARG:HH11	1:D:394:ARG:HG3	1.48	0.77
1:A:381:LYS:HB3	6:A:2578:HOH:O	1.84	0.77
1:C:167[B]:ASN:ND2	1:C:911:PRO:HA	2.00	0.76
1:B:921:ILE:HG13	6:B:2754:HOH:O	1.86	0.76
1:D:343:THR:HA	4:D:1031:FAD:HM73	1.69	0.75
1:B:167[B]:ASN:ND2	1:B:911:PRO:HA	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410[A]:ARG:HG3	6:C:2607:HOH:O	1.86	0.75
1:D:634:ASP:OD1	6:D:2891:HOH:O	2.04	0.75
1:A:343:THR:HA	4:A:1031:FAD:HM73	1.68	0.74
1:A:662:ALA:HA	6:A:2822:HOH:O	1.87	0.74
1:C:907:LEU:CD2	1:C:907:LEU:H	2.00	0.74
1:C:938:LEU:HD23	6:C:3080:HOH:O	1.88	0.74
1:C:378:GLU:HA	6:C:2584:HOH:O	1.88	0.74
1:D:978:HIS:HA	6:D:3200:HOH:O	1.85	0.74
1:C:950:GLU:HG2	6:C:3130:HOH:O	1.89	0.73
1:C:391:LEU:HA	1:C:410[B]:ARG:HH12	1.53	0.73
1:B:343:THR:HA	4:B:1031:FAD:HM73	1.69	0.72
1:C:779[B]:THR:HG21	1:C:932[B]:LEU:CD2	2.19	0.72
1:D:66:THR:HG22	6:D:3105:HOH:O	1.89	0.72
1:D:677:GLU:O	1:D:678:ARG:HB2	1.90	0.72
1:B:395:LYS:HG3	1:B:407:GLN:NE2	2.05	0.71
1:D:263:GLU:OE1	1:D:449:GLU:HG2	1.90	0.71
1:A:883:LEU:HG	1:A:887:LYS:HE3	1.70	0.71
1:A:893:GLU:OE1	1:A:896:ARG:NH2	2.24	0.71
1:B:408:PHE:HB3	1:B:410[B]:ARG:HH22	1.54	0.71
1:C:143:TYR:O	1:D:861:LYS:HE2	1.92	0.70
1:A:22:THR:HB	6:A:2054:HOH:O	1.91	0.70
1:B:952:MET:HG2	6:B:3039:HOH:O	1.90	0.70
1:C:820:GLN:HA	6:D:3190:HOH:O	1.92	0.69
1:D:1019:LEU:HD23	1:D:1019:LEU:N	2.06	0.69
1:A:863:LYS:HA	6:A:3008:HOH:O	1.93	0.69
1:A:622:CYS:SG	6:A:2851:HOH:O	2.51	0.69
6:A:2811:HOH:O	1:B:2:ALA:HB1	1.93	0.69
1:C:251:LEU:HB3	6:C:2337:HOH:O	1.93	0.69
1:C:331:ILE:HG23	1:C:433:VAL:HG21	1.76	0.68
1:C:703:GLN:HG3	6:C:2878:HOH:O	1.92	0.68
1:B:409:VAL:C	1:B:410[B]:ARG:NE	2.47	0.68
1:C:448:LYS:HE2	6:C:2648:HOH:O	1.94	0.68
1:C:391:LEU:HG	1:C:410[B]:ARG:NH1	2.09	0.68
1:D:315:LYS:HD2	1:D:322:CYS:HB2	1.76	0.67
1:B:845:GLU:HG3	1:B:912:PHE:CE2	2.29	0.67
1:D:395:LYS:HD2	1:D:407:GLN:NE2	2.10	0.67
1:B:414:ASP:OD1	6:B:2652:HOH:O	2.12	0.67
1:A:861:LYS:HE2	1:B:143:TYR:O	1.94	0.67
1:B:391:LEU:HD21	1:B:410[B]:ARG:HH12	1.58	0.67
1:C:907:LEU:HD23	1:C:907:LEU:H	1.58	0.67
1:D:172:ARG:HB2	6:D:2333:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410[B]:ARG:HD2	1:B:425:GLN:O	1.94	0.66
1:A:397:ILE:HD12	1:A:428:HIS:HE1	1.61	0.66
1:B:952:MET:HE3	6:B:3039:HOH:O	1.93	0.66
1:A:634:ASP:OD2	6:A:2819:HOH:O	2.14	0.66
1:B:442:LEU:HD22	1:B:482:ILE:HD11	1.76	0.66
1:C:326:SER:HB3	6:C:2497:HOH:O	1.95	0.66
1:C:164:LYS:CG	1:C:909:ARG:HH12	2.08	0.66
1:D:442:LEU:HD22	1:D:482:ILE:HD11	1.78	0.66
1:C:207:ALA:HB1	6:C:2337:HOH:O	1.94	0.66
1:C:164:LYS:HG3	1:C:909:ARG:HH12	1.61	0.66
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.77	0.66
1:A:402:ARG:HG2	1:A:402:ARG:NH1	2.11	0.65
1:A:402:ARG:HG2	1:A:402:ARG:HH11	1.61	0.65
1:B:518:LYS:HE3	6:B:2739:HOH:O	1.94	0.65
1:C:872:MET:HE1	6:C:3016:HOH:O	1.97	0.65
1:A:50:PHE:HE2	1:B:369:ASN:HA	1.60	0.65
1:A:856:THR:HG23	6:A:3001:HOH:O	1.96	0.65
1:C:410[B]:ARG:NE	1:C:427:VAL:HG23	2.11	0.65
1:A:927:LYS:HB3	6:A:3059:HOH:O	1.97	0.65
1:B:722:ARG:O	1:B:726:GLU:HG3	1.97	0.64
1:D:394:ARG:HD2	1:D:409:VAL:CG1	2.27	0.64
1:B:167[B]:ASN:ND2	1:B:910:LYS:O	2.31	0.64
1:D:36:LEU:HD23	6:D:2113:HOH:O	1.98	0.64
1:A:448:LYS:HE2	6:A:2648:HOH:O	1.97	0.64
1:D:178:SER:HB3	6:D:2340:HOH:O	1.97	0.63
1:D:376:GLU:HB2	6:D:2657:HOH:O	1.98	0.63
1:A:173:ASN:HD22	1:A:174:PRO:HD2	1.63	0.63
1:B:831:CYS:O	6:B:3001:HOH:O	2.15	0.63
1:B:872:MET:HE3	6:B:3054:HOH:O	1.97	0.62
1:A:293:ILE:CD1	1:A:393:PRO:HB2	2.29	0.62
1:D:722:ARG:O	1:D:726:GLU:HG3	1.99	0.62
1:B:875:LYS:HE2	6:B:3133:HOH:O	1.99	0.62
1:C:13:GLU:HB2	6:C:2018:HOH:O	1.98	0.62
1:D:379:LEU:HD23	6:D:2663:HOH:O	1.99	0.62
1:A:786:PRO:HB3	1:D:942:GLU:HA	1.82	0.62
1:D:984:ASP:HB3	6:D:3220:HOH:O	1.99	0.62
1:C:907:LEU:CD2	1:C:907:LEU:N	2.62	0.62
1:D:901:ASN:HD22	1:D:901:ASN:N	1.96	0.62
1:C:845:GLU:HG3	1:C:912:PHE:CE2	2.34	0.61
1:B:12:ILE:O	1:B:15:ILE:HG22	2.00	0.61
1:C:22:THR:HB	6:C:2056:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:783:ARG:HD3	6:D:3029:HOH:O	2.00	0.61
1:B:408:PHE:HB2	1:B:410[B]:ARG:NH2	2.16	0.61
1:B:981:THR:HG23	6:B:3167:HOH:O	2.00	0.61
1:C:410[A]:ARG:HG2	1:C:411:THR:N	2.15	0.61
6:C:3080:HOH:O	1:D:759:ARG:HB2	1.99	0.61
1:A:637:VAL:HB	6:A:2822:HOH:O	1.99	0.61
1:A:722:ARG:O	1:A:726:GLU:HG3	2.00	0.61
1:B:845:GLU:HG3	1:B:912:PHE:CD2	2.35	0.61
1:D:394:ARG:NH1	1:D:409:VAL:HG21	2.15	0.61
1:B:416:THR:OG1	1:B:416:THR:O	2.18	0.60
1:C:722:ARG:O	1:C:726:GLU:HG3	2.01	0.60
1:C:408:PHE:HB2	1:C:410[B]:ARG:NH2	2.16	0.60
1:A:287:GLU:HG2	6:A:2454:HOH:O	2.02	0.60
1:A:865:VAL:HG13	6:A:3029:HOH:O	2.00	0.60
1:D:63:LYS:HB2	6:D:2172:HOH:O	2.02	0.59
1:A:485:MET:HE3	6:A:2315:HOH:O	2.01	0.59
1:A:410:ARG:HG2	1:A:411:THR:N	2.16	0.59
1:D:5:LEU:HD23	6:D:2001:HOH:O	2.01	0.59
1:A:173:ASN:HD22	1:A:174:PRO:CD	2.15	0.59
1:B:414:ASP:OD1	1:B:418:LYS:HB2	2.02	0.59
1:D:673:HIS:CG	1:D:675:MET:HG2	2.38	0.59
1:D:474:PRO:HG2	6:D:2345:HOH:O	2.03	0.59
1:D:995:VAL:HB	6:D:3187:HOH:O	2.03	0.59
1:A:293:ILE:HD11	1:A:393:PRO:HB2	1.85	0.58
6:C:3080:HOH:O	1:D:759:ARG:HD3	2.01	0.58
1:B:61:ASP:HB2	6:B:2070:HOH:O	2.03	0.58
1:C:497:LYS:HE2	1:D:27:ALA:O	2.03	0.58
1:A:273:GLU:HB3	6:A:2441:HOH:O	2.03	0.58
1:D:958:LYS:NZ	6:D:3187:HOH:O	2.35	0.58
1:A:52:CYS:HB3	1:A:384:LYS:HG2	1.85	0.58
1:A:378:GLU:CD	6:A:2578:HOH:O	2.42	0.58
1:B:408:PHE:CB	1:B:410[B]:ARG:HH22	2.12	0.58
1:D:167:ASN:HB3	6:D:3137:HOH:O	2.04	0.58
1:B:263:GLU:OE1	1:B:449:GLU:HG2	2.03	0.58
1:B:856:THR:HG23	6:B:3033:HOH:O	2.03	0.58
1:C:845:GLU:HG3	1:C:912:PHE:CD2	2.38	0.58
1:D:328:LEU:HD12	6:D:2153:HOH:O	2.04	0.58
1:B:917:PRO:HA	6:B:3087:HOH:O	2.04	0.57
1:A:660:SER:HB3	6:A:2851:HOH:O	2.04	0.57
6:C:2909:HOH:O	1:D:775[A]:LEU:HD12	2.04	0.57
1:C:52:CYS:HB2	1:C:384:LYS:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:PHE:HE1	1:D:367:PHE:HE1	1.51	0.57
1:C:395:LYS:HD2	1:C:407:GLN:NE2	2.18	0.57
6:C:2192:HOH:O	1:D:29:HIS:HB2	2.03	0.57
1:A:497:LYS:HE2	1:B:27:ALA:O	2.05	0.57
1:C:391:LEU:HG	1:C:410[B]:ARG:HH12	1.67	0.57
1:C:408:PHE:CB	1:C:410[B]:ARG:NH2	2.67	0.57
1:D:899:GLU:O	1:D:899:GLU:HG2	2.02	0.57
1:D:673:HIS:CD2	1:D:675:MET:HG2	2.38	0.57
1:D:900:GLN:HG2	1:D:901:ASN:H	1.69	0.57
1:B:948:ILE:HG12	1:B:1002:ILE:HG12	1.85	0.57
1:B:173:ASN:HB3	1:B:176:LEU:HG	1.87	0.57
1:B:367:PHE:HE1	1:B:387:PHE:CB	2.17	0.57
1:B:414:ASP:CG	6:B:2652:HOH:O	2.43	0.57
1:C:978:HIS:HE1	1:D:84:ASP:OD2	1.86	0.57
1:D:872:MET:HE2	6:D:3181:HOH:O	2.04	0.57
1:A:872:MET:HE1	6:A:2998:HOH:O	2.05	0.57
1:B:952:MET:O	1:B:998:ILE:HD13	2.05	0.57
1:D:410:ARG:HG2	1:D:411:THR:N	2.20	0.57
1:A:39:LYS:HG3	6:A:2084:HOH:O	2.04	0.56
1:C:783:ARG:HD3	6:D:3013:HOH:O	2.05	0.56
1:A:859:HIS:HD2	1:A:862:GLY:N	1.99	0.56
1:B:954:ILE:CG2	1:B:998:ILE:HD11	2.31	0.56
1:D:673:HIS:CD2	1:D:675:MET:N	2.54	0.56
1:D:959:CYS:O	1:D:962[B]:THR:HG22	2.05	0.56
1:D:36:LEU:HG	6:D:2110:HOH:O	2.05	0.56
1:B:859:HIS:HA	1:B:865:VAL:HG23	1.88	0.56
1:C:775:LEU:HD12	6:D:2990:HOH:O	2.04	0.56
1:D:1007:ARG:HG2	6:D:3247:HOH:O	2.06	0.56
1:C:907:LEU:N	1:C:907:LEU:HD22	2.21	0.56
1:A:1014:LYS:HB3	6:A:3159:HOH:O	2.06	0.56
1:A:391:LEU:HD22	1:A:408:PHE:CB	2.36	0.56
1:B:115:MET:HE1	6:B:2996:HOH:O	2.06	0.56
1:B:577[B]:SER:HB2	6:B:2797:HOH:O	2.06	0.56
1:C:505:LYS:HE2	6:C:2692:HOH:O	2.05	0.56
1:B:22:THR:HA	6:B:2064:HOH:O	2.05	0.56
1:A:485:MET:HE1	1:B:32:LEU:HB2	1.87	0.56
1:B:777:ALA:HA	6:B:2956:HOH:O	2.05	0.56
1:C:407:GLN:HG2	6:C:2604:HOH:O	2.06	0.56
1:A:172:ARG:HD2	6:A:2318:HOH:O	2.04	0.55
1:B:409:VAL:CA	1:B:410[B]:ARG:HE	2.19	0.55
1:D:52:CYS:HB3	1:D:384:LYS:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:990:THR:O	1:D:990:THR:HG22	2.06	0.55
1:A:12:ILE:O	1:A:15:ILE:HG22	2.06	0.55
1:C:327:PRO:O	1:C:328:LEU:C	2.43	0.55
1:C:36:LEU:HG	6:C:2082:HOH:O	2.07	0.55
1:D:363:PHE:HE1	1:D:367:PHE:CE1	2.25	0.55
1:D:52:CYS:HB3	1:D:384:LYS:CG	2.36	0.55
1:C:410[B]:ARG:HG2	1:C:425:GLN:O	2.06	0.55
1:D:677:GLU:HG2	1:D:678:ARG:H	1.72	0.55
1:D:783:ARG:NH1	6:D:3029:HOH:O	2.38	0.55
1:A:990:THR:O	1:A:990:THR:HG22	2.07	0.55
1:A:775:LEU:HD12	6:B:2932:HOH:O	2.07	0.55
1:A:777:ALA:HA	6:A:2924:HOH:O	2.06	0.55
1:B:954:ILE:HG23	1:B:998:ILE:CD1	2.33	0.55
1:B:391:LEU:CG	1:B:410[B]:ARG:HH12	2.19	0.54
1:B:787:GLY:N	6:B:2969:HOH:O	2.39	0.54
1:B:394:ARG:NH2	1:B:423:GLU:OE2	2.40	0.54
1:C:796:ILE:HD13	1:C:813:LEU:HB3	1.88	0.54
1:C:842:SER:HA	1:C:916:LYS:HG2	1.90	0.54
1:C:857:GLU:HG3	6:C:3012:HOH:O	2.06	0.54
1:D:394:ARG:HD2	1:D:409:VAL:HG11	1.88	0.54
1:B:395:LYS:HG3	1:B:407:GLN:HE21	1.72	0.54
1:B:409:VAL:C	1:B:410[B]:ARG:HH21	2.11	0.54
1:D:458:ARG:HG3	6:D:2716:HOH:O	2.07	0.54
1:B:990:THR:O	1:B:990:THR:HG22	2.08	0.54
1:D:900:GLN:HG2	1:D:901:ASN:N	2.22	0.54
1:A:471:THR:HG22	6:A:2651:HOH:O	2.07	0.54
1:B:391:LEU:HD23	1:B:408:PHE:CB	2.38	0.54
1:B:364:ARG:HA	1:B:391:LEU:O	2.08	0.54
1:D:394:ARG:HD2	1:D:409:VAL:HG13	1.90	0.53
1:D:859:HIS:HA	1:D:865:VAL:HG23	1.90	0.53
1:B:367:PHE:HE1	1:B:387:PHE:HB3	1.73	0.53
1:D:680:MET:HE3	1:D:688:PRO:HD2	1.90	0.53
1:B:796:ILE:HD13	1:B:813:LEU:HB3	1.90	0.53
1:C:943:GLN:HB3	6:D:2844:HOH:O	2.08	0.53
1:D:948:ILE:HG12	1:D:1002:ILE:HG12	1.90	0.53
1:C:378:GLU:CD	6:C:2584:HOH:O	2.47	0.53
1:D:885:GLN:HG2	6:D:2580:HOH:O	2.09	0.53
1:A:886:ARG:NH2	6:A:3029:HOH:O	2.34	0.53
1:A:935:PHE:CE2	1:B:612:LEU:HD11	2.43	0.53
1:C:164:LYS:HG3	1:C:909:ARG:NH1	2.24	0.53
1:C:418:LYS:HD3	1:C:420:ASN:OD1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:GLN:HG3	6:D:2341:HOH:O	2.09	0.53
1:C:27:ALA:O	1:D:497:LYS:HE2	2.09	0.53
1:A:173:ASN:ND2	1:A:175:CYS:SG	2.81	0.53
1:D:364:ARG:HA	1:D:391:LEU:O	2.09	0.53
1:B:681:GLY:C	1:B:682:LEU:HD12	2.30	0.53
1:B:776:ARG:NH1	6:B:2956:HOH:O	2.41	0.53
1:D:391:LEU:HD22	1:D:408:PHE:CG	2.44	0.53
1:D:673:HIS:CD2	1:D:674:GLY:N	2.77	0.53
1:B:682:LEU:HD12	1:B:682:LEU:N	2.24	0.52
1:C:955:ASN:HB3	1:C:978:HIS:HB3	1.89	0.52
1:D:164:LYS:HE2	6:D:3135:HOH:O	2.09	0.52
1:D:753:ALA:HB3	6:D:3003:HOH:O	2.09	0.52
1:A:796:ILE:HD13	1:A:813:LEU:HB3	1.92	0.52
1:D:680:MET:CE	1:D:688:PRO:HD2	2.39	0.52
1:D:52:CYS:HB2	6:D:2668:HOH:O	2.08	0.52
1:A:776:ARG:NH1	6:A:2924:HOH:O	2.43	0.52
1:B:577[A]:SER:HB3	6:B:2797:HOH:O	2.10	0.52
1:C:32:LEU:HB2	1:D:485:MET:HE1	1.91	0.52
1:D:394:ARG:CG	1:D:394:ARG:HH11	2.19	0.52
1:D:3:PRO:HD2	6:D:2001:HOH:O	2.10	0.52
1:B:52:CYS:HB3	6:B:2633:HOH:O	2.09	0.52
1:C:12:ILE:O	1:C:15:ILE:HG22	2.10	0.52
1:C:612:LEU:HD11	1:D:935:PHE:CE2	2.45	0.52
1:C:47:LYS:HD3	1:D:373:VAL:HG12	1.90	0.52
1:A:397:ILE:HD12	1:A:428:HIS:CE1	2.43	0.52
1:A:828:GLN:HG2	6:A:2962:HOH:O	2.09	0.52
1:C:390:PHE:O	1:C:410[B]:ARG:NH1	2.42	0.52
1:C:828:GLN:HG2	6:C:2974:HOH:O	2.09	0.52
1:D:651:MET:HE3	1:D:700:GLN:HG3	1.91	0.52
1:A:378:GLU:HA	6:A:2578:HOH:O	2.09	0.52
1:A:520:GLU:HG2	6:A:2708:HOH:O	2.09	0.52
1:A:842:SER:HA	1:A:916:LYS:HG2	1.92	0.52
1:C:309:PHE:CE1	1:C:331:ILE:HD11	2.44	0.52
1:C:682:LEU:HD12	1:C:682:LEU:N	2.25	0.52
1:B:52:CYS:HB2	1:B:384:LYS:HB2	1.92	0.52
1:D:410:ARG:HG3	6:D:2684:HOH:O	2.10	0.52
1:A:552:ALA:HB3	1:A:553:PRO:HD3	1.91	0.51
1:C:908:GLU:O	1:C:909:ARG:C	2.48	0.51
1:C:990:THR:O	1:C:990:THR:HG22	2.10	0.51
1:D:859:HIS:HD2	1:D:862:GLY:N	2.03	0.51
1:A:341:GLY:HA3	1:A:371:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:PRO:HB3	6:B:2754:HOH:O	2.09	0.51
1:A:948:ILE:HG12	1:A:1002:ILE:HG12	1.92	0.51
1:A:911:PRO:HB3	6:A:2301:HOH:O	2.09	0.51
1:C:373:VAL:HG12	1:D:47:LYS:HD3	1.91	0.51
1:A:923:ASP:OD1	1:D:937:GLU:HG2	2.10	0.51
1:A:612:LEU:HD11	1:B:935:PHE:CE2	2.45	0.51
1:B:842:SER:HA	1:B:916:LYS:HG2	1.91	0.51
1:C:179:GLN:HG3	6:C:2302:HOH:O	2.11	0.51
1:C:859:HIS:HA	1:C:865:VAL:HG23	1.93	0.51
1:D:1007:ARG:CD	1:D:1011:TYR:HB2	2.40	0.51
1:D:828:GLN:HG2	6:D:3062:HOH:O	2.10	0.51
1:D:922:LYS:HE3	6:D:3149:HOH:O	2.10	0.51
1:B:193:LEU:HD23	1:B:281:ILE:HD13	1.92	0.51
1:B:362:VAL:HG13	1:B:391:LEU:HD13	1.93	0.51
1:C:783:ARG:NH1	6:D:3013:HOH:O	2.42	0.51
1:D:486:ALA:HB1	1:D:491:GLU:OE1	2.10	0.51
1:B:378:GLU:CD	6:B:2627:HOH:O	2.48	0.51
1:A:241:VAL:O	1:A:245[B]:ILE:HG12	2.11	0.51
1:C:364:ARG:HA	1:C:391:LEU:O	2.11	0.51
1:C:582:ILE:HD11	1:D:1015:ARG:CZ	2.41	0.51
1:B:1018:PRO:HD3	6:B:3208:HOH:O	2.09	0.51
1:C:29:HIS:HB2	6:D:2231:HOH:O	2.10	0.51
1:D:12:ILE:O	1:D:15:ILE:HG22	2.10	0.51
1:D:673:HIS:HD2	1:D:674:GLY:N	2.08	0.51
1:C:324:CYS:O	1:C:325:HIS:HB2	2.11	0.51
1:A:577:SER:HB2	6:A:2765:HOH:O	2.10	0.50
1:A:859:HIS:HA	1:A:865:VAL:HG23	1.92	0.50
6:A:2200:HOH:O	1:B:29:HIS:HB2	2.11	0.50
1:B:451:LEU:O	1:B:454:ILE:HG12	2.10	0.50
1:C:115:MET:HE1	6:C:2976:HOH:O	2.11	0.50
1:C:893:GLU:OE2	1:C:896:ARG:NH2	2.45	0.50
1:B:849:TRP:CH2	1:B:854:PRO:HG3	2.46	0.50
1:C:391:LEU:HD23	1:C:408:PHE:CB	2.41	0.50
1:C:53:GLU:OE1	1:C:54:LYS:N	2.44	0.50
1:C:859:HIS:HD2	1:C:862:GLY:N	2.04	0.50
1:D:673:HIS:CE1	1:D:679:GLY:HA3	2.46	0.50
1:A:44:ASN:HB2	1:A:45:PRO:CD	2.41	0.50
1:C:874:LYS:HD3	6:C:3032:HOH:O	2.12	0.50
1:D:378:GLU:HG3	6:D:2663:HOH:O	2.10	0.50
1:C:36:LEU:HD23	6:C:2086:HOH:O	2.11	0.50
1:D:505:LYS:HD2	6:D:2752:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:909:ARG:NH1	6:D:3135:HOH:O	2.44	0.50
1:A:394:ARG:HG3	1:A:409:VAL:HG13	1.94	0.50
1:B:358:ARG:NH2	6:B:2586:HOH:O	2.44	0.50
1:B:954:ILE:HG12	1:B:998:ILE:HD11	1.93	0.50
1:D:901:ASN:ND2	1:D:901:ASN:N	2.60	0.50
1:B:367:PHE:CE1	1:B:387:PHE:CB	2.93	0.50
1:A:179:GLN:HG3	6:A:2319:HOH:O	2.11	0.50
1:B:828:GLN:HG3	6:B:2996:HOH:O	2.12	0.50
1:A:29:HIS:HB2	6:B:2229:HOH:O	2.12	0.50
1:B:82:CYS:O	1:B:98:LYS:HD2	2.11	0.50
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.93	0.50
1:D:911:PRO:HG3	6:D:2157:HOH:O	2.11	0.50
1:C:22:THR:HA	6:C:2055:HOH:O	2.12	0.49
1:A:947[A]:VAL:HG12	1:A:1003:ARG:O	2.11	0.49
1:A:364:ARG:HA	1:A:391:LEU:O	2.11	0.49
1:D:263:GLU:O	1:D:264:ASN:HB2	2.11	0.49
1:A:787:GLY:HA3	1:D:942:GLU:OE2	2.12	0.49
1:D:951:GLU:CD	6:D:3181:HOH:O	2.50	0.49
1:C:261:LEU:HD21	1:C:451:LEU:HD21	1.95	0.49
1:D:552:ALA:HB3	1:D:553:PRO:HD3	1.93	0.49
1:D:962[A]:THR:HG21	1:D:991:LEU:HB3	1.93	0.49
1:A:859:HIS:CD2	1:A:862:GLY:H	2.17	0.49
1:B:391:LEU:CD2	1:B:410[B]:ARG:NH1	2.70	0.49
1:B:699:ARG:HA	1:B:699:ARG:NE	2.27	0.49
1:C:391:LEU:CD2	1:C:410[B]:ARG:NH2	2.72	0.49
1:C:281[B]:ILE:HD13	1:C:451:LEU:HD22	1.93	0.49
1:D:796:ILE:HD13	1:D:813:LEU:HB3	1.95	0.49
1:A:144:ALA:O	1:B:861:LYS:HG2	2.12	0.49
1:D:677:GLU:O	1:D:678:ARG:CB	2.60	0.49
1:D:678:ARG:HG3	1:D:679:GLY:N	2.28	0.49
1:B:574:LYS:HB3	1:B:614:SER:HB2	1.94	0.49
1:C:219:LYS:HG3	1:C:260:SER:OG	2.12	0.49
1:C:311:PRO:O	1:C:315:LYS:HG3	2.13	0.49
1:C:408:PHE:C	1:C:410[B]:ARG:HH21	2.16	0.49
1:D:1007:ARG:HD3	1:D:1011:TYR:HB2	1.95	0.49
1:D:962[A]:THR:HG23	6:D:3190:HOH:O	2.12	0.49
1:A:612:LEU:HA	6:A:2798:HOH:O	2.12	0.49
1:B:219:LYS:HG3	1:B:260:SER:OG	2.12	0.49
1:D:678:ARG:NH1	6:D:2945:HOH:O	2.46	0.49
1:A:955:ASN:HB3	1:A:978:HIS:HB3	1.94	0.48
1:B:952:MET:O	1:B:998:ILE:CD1	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:ARG:HD3	1:D:422:ASP:OD2	2.12	0.48
1:B:828:GLN:HG2	6:B:2997:HOH:O	2.11	0.48
1:B:672:PRO:HA	1:B:682:LEU:O	2.14	0.48
1:A:82:CYS:O	1:A:98:LYS:HD2	2.13	0.48
1:B:410[A]:ARG:HG2	1:B:411:THR:N	2.27	0.48
1:D:939:SER:OG	1:D:941:ILE:HG12	2.13	0.48
1:C:132:THR:HB	1:C:137:VAL:HG23	1.94	0.48
1:C:241:VAL:O	1:C:245[B]:ILE:HG12	2.13	0.48
1:C:413:GLN:HG3	1:C:419:TRP:CE2	2.48	0.48
6:C:2976:HOH:O	1:D:22:THR:HG23	2.13	0.48
1:A:263:GLU:O	1:A:264:ASN:HB2	2.12	0.48
1:B:420:ASN:ND2	6:B:2650:HOH:O	2.47	0.48
1:D:863:LYS:HE2	6:D:2172:HOH:O	2.12	0.48
1:C:916:LYS:HE3	6:C:2988:HOH:O	2.12	0.48
1:C:191:ALA:O	1:C:279:ALA:HA	2.14	0.48
1:A:54:LYS:HE3	1:A:56:GLU:HB3	1.95	0.48
1:A:896:ARG:O	1:A:900:GLN:HG3	2.13	0.48
1:C:486:ALA:HB1	1:C:491:GLU:OE1	2.14	0.48
1:D:346:ASP:OD2	4:D:1031:FAD:H6	2.13	0.48
1:A:875:LYS:HB3	6:A:3018:HOH:O	2.14	0.48
1:C:338:LEU:HD23	1:C:362:VAL:HB	1.94	0.48
1:A:734:ALA:HA	1:A:735:THR:HA	1.57	0.47
1:B:18:LEU:HD13	6:B:3156:HOH:O	2.14	0.47
1:B:887:LYS:HD2	6:B:2550:HOH:O	2.14	0.47
1:C:164:LYS:HG2	1:C:909:ARG:HH12	1.79	0.47
1:D:621:TRP:O	1:D:625:VAL:HG23	2.14	0.47
1:B:505:LYS:HE2	6:B:2722:HOH:O	2.13	0.47
1:C:978:HIS:HD2	6:D:2291:HOH:O	1.96	0.47
1:B:191:ALA:O	1:B:279:ALA:HA	2.15	0.47
1:B:656:LYS:HD2	6:B:2869:HOH:O	2.14	0.47
1:C:334:ALA:HA	6:C:2549:HOH:O	2.14	0.47
1:A:660:SER:CB	6:A:2851:HOH:O	2.61	0.47
1:A:874:LYS:HG2	6:A:3015:HOH:O	2.14	0.47
1:A:959:CYS:O	1:A:962[B]:THR:HG22	2.14	0.47
1:B:394:ARG:HG3	1:B:409:VAL:CG1	2.40	0.47
1:B:448:LYS:HD3	6:B:2681:HOH:O	2.14	0.47
1:D:36:LEU:HB3	6:D:2117:HOH:O	2.14	0.47
1:D:779[B]:THR:CG2	1:D:932:LEU:HD22	2.27	0.47
1:D:962[A]:THR:CG2	1:D:991:LEU:HB3	2.45	0.47
1:A:356:ALA:O	6:A:2542:HOH:O	2.20	0.47
1:C:44:ASN:HB2	1:C:45:PRO:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:MET:HE1	1:D:32:LEU:HB2	1.96	0.47
1:D:779[B]:THR:HG23	1:D:929:LEU:CD2	2.45	0.47
1:A:191:ALA:O	1:A:279:ALA:HA	2.14	0.47
1:B:409:VAL:O	1:B:410[B]:ARG:NH2	2.47	0.47
1:B:845:GLU:HG3	1:B:912:PHE:CZ	2.50	0.47
1:C:574:LYS:HB3	1:C:614:SER:HB2	1.97	0.47
1:D:673:HIS:CD2	1:D:673:HIS:C	2.88	0.47
1:D:947[B]:VAL:HG22	1:D:1003:ARG:O	2.15	0.47
1:D:82:CYS:O	1:D:98:LYS:HD2	2.14	0.47
1:C:52:CYS:HB2	1:C:383:GLU:O	2.15	0.47
1:C:393:PRO:HD3	6:C:2594:HOH:O	2.14	0.47
1:C:54:LYS:HG3	6:C:2117:HOH:O	2.15	0.47
1:C:935:PHE:CE2	1:D:612:LEU:HD11	2.49	0.47
1:A:1015:ARG:CZ	1:B:582:ILE:HD11	2.45	0.47
1:B:367:PHE:CE1	1:B:387:PHE:HB2	2.49	0.47
1:B:911:PRO:HG2	6:B:2436:HOH:O	2.14	0.47
1:C:870:GLU:O	1:C:889:ILE:HD13	2.15	0.47
1:D:955:ASN:HB3	1:D:978:HIS:HB3	1.96	0.47
1:B:696:ARG:NH1	6:B:2901:HOH:O	2.29	0.46
1:B:744:LEU:HD21	6:B:2460:HOH:O	2.15	0.46
1:B:193:LEU:HD22	1:B:193:LEU:N	2.30	0.46
1:B:311:PRO:O	1:B:315:LYS:HG3	2.14	0.46
1:B:417:GLY:O	1:B:418:LYS:C	2.53	0.46
1:B:486:ALA:HB1	1:B:491:GLU:OE1	2.16	0.46
1:C:908:GLU:C	1:C:909:ARG:O	2.51	0.46
1:B:340:ALA:N	6:B:2562:HOH:O	2.47	0.46
1:C:734:ALA:HA	1:C:735:THR:HA	1.57	0.46
1:D:892:GLU:HG3	6:D:3132:HOH:O	2.14	0.46
1:A:934:THR:OG1	1:A:937:GLU:HG3	2.15	0.46
1:B:358:ARG:NH2	6:B:2587:HOH:O	2.48	0.46
1:B:552:ALA:HB3	1:B:553:PRO:HD3	1.97	0.46
1:D:379:LEU:O	1:D:383:GLU:HG3	2.15	0.46
1:B:346:ASP:OD2	4:B:1031:FAD:H6	2.16	0.46
1:C:408:PHE:HB3	1:C:410[B]:ARG:HH22	1.81	0.46
1:B:409:VAL:C	1:B:410[B]:ARG:NH2	2.69	0.46
1:B:693:ASN:HA	1:B:696:ARG:HD3	1.97	0.46
1:A:864:PRO:HD3	6:A:3008:HOH:O	2.14	0.46
1:C:391:LEU:CD2	1:C:408:PHE:CB	2.93	0.46
1:C:409:VAL:C	1:C:410[B]:ARG:CZ	2.84	0.46
1:D:315:LYS:NZ	6:D:2572:HOH:O	2.48	0.46
1:A:413:GLN:HG3	1:A:419:TRP:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:LEU:HD13	1:B:638:ILE:HB	1.97	0.46
1:B:688:PRO:HG3	1:B:720:ILE:HD13	1.97	0.46
1:B:870:GLU:O	1:B:889:ILE:HD13	2.16	0.46
1:C:642:MET:HE2	6:C:2755:HOH:O	2.15	0.46
1:A:193:LEU:HD22	1:A:193:LEU:N	2.31	0.46
1:A:688:PRO:HG3	1:A:720:ILE:HD13	1.96	0.46
1:A:7:LYS:NZ	6:A:2014:HOH:O	2.41	0.46
1:C:861:LYS:HD2	6:D:2292:HOH:O	2.15	0.46
1:D:394:ARG:CG	1:D:394:ARG:NH1	2.78	0.46
1:D:673:HIS:ND1	1:D:690:LEU:HD11	2.31	0.46
1:A:379:LEU:O	1:A:383:GLU:HG3	2.16	0.46
1:C:409:VAL:C	1:C:410[B]:ARG:NH2	2.70	0.46
1:A:219:LYS:HG3	1:A:260:SER:OG	2.15	0.45
1:C:696:ARG:HH11	1:C:696:ARG:HG3	1.81	0.45
1:D:338:LEU:HD23	1:D:362:VAL:HB	1.98	0.45
1:B:36:LEU:HD23	6:B:2105:HOH:O	2.15	0.45
1:D:191:ALA:O	1:D:279:ALA:HA	2.16	0.45
1:A:346:ASP:OD2	4:A:1031:FAD:H6	2.15	0.45
1:D:872:MET:CE	6:D:3181:HOH:O	2.64	0.45
1:A:844:GLU:HA	1:A:847:GLN:HE21	1.82	0.45
6:A:2805:HOH:O	1:B:1014:LYS:HD3	2.16	0.45
1:B:955:ASN:HB3	1:B:978:HIS:HB3	1.97	0.45
1:C:124:LEU:HD13	1:C:160:SER:HB2	1.98	0.45
1:C:621:TRP:O	1:C:625:VAL:HG23	2.17	0.45
1:D:941:ILE:N	1:D:941:ILE:HD13	2.31	0.45
1:C:947[B]:VAL:HG12	1:C:1003:ARG:O	2.17	0.45
1:A:1007:ARG:HD3	1:A:1011:TYR:HB2	1.98	0.45
1:B:416:THR:N	6:B:2652:HOH:O	2.41	0.45
1:C:1007:ARG:HD3	1:C:1011:TYR:HB2	1.99	0.45
1:D:193:LEU:HD22	1:D:193:LEU:N	2.32	0.45
1:A:760:THR:HG23	1:B:932[A]:LEU:HD23	1.99	0.45
1:B:167[B]:ASN:ND2	6:B:2320:HOH:O	2.50	0.45
1:C:897:LEU:HD23	1:C:900:GLN:OE1	2.17	0.45
1:C:167[B]:ASN:HD22	1:C:911:PRO:HA	1.76	0.45
1:A:393:PRO:HD3	6:A:2590:HOH:O	2.15	0.45
1:A:53:GLU:HG2	1:A:53:GLU:O	2.16	0.45
1:B:44:ASN:HB2	1:B:45:PRO:CD	2.47	0.45
1:C:696:ARG:HD2	6:C:2868:HOH:O	2.16	0.45
1:D:191:ALA:HB2	1:D:276:TYR:CD2	2.52	0.45
1:A:223:VAL:HG23	6:A:2389:HOH:O	2.17	0.45
1:B:705:PRO:HA	1:B:730:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410[B]:ARG:HE	1:C:427:VAL:HG23	1.81	0.45
1:C:859:HIS:CD2	1:C:862:GLY:H	2.19	0.45
1:A:27:ALA:O	1:B:497:LYS:HE2	2.17	0.44
1:B:391:LEU:HG	1:B:410[B]:ARG:HH12	1.81	0.44
1:B:691:VAL:HG21	1:B:720:ILE:HG23	2.00	0.44
1:C:193:LEU:HD22	1:C:193:LEU:N	2.32	0.44
1:A:223:VAL:HG23	1:A:245[A]:ILE:CD1	2.47	0.44
1:A:318:LYS:HB3	6:A:2503:HOH:O	2.17	0.44
1:B:39:LYS:HG3	6:B:2108:HOH:O	2.17	0.44
1:D:451:LEU:O	1:D:454:ILE:HG12	2.17	0.44
1:D:849:TRP:CH2	1:D:854:PRO:HG3	2.52	0.44
1:B:409:VAL:N	1:B:410[B]:ARG:NH2	2.59	0.44
1:B:893:GLU:O	1:B:897:LEU:HG	2.17	0.44
1:C:394:ARG:HD3	1:C:394:ARG:HA	1.75	0.44
1:C:688:PRO:HG3	1:C:720:ILE:HD13	1.99	0.44
1:C:893:GLU:OE2	1:C:896:ARG:CZ	2.65	0.44
1:B:417:GLY:O	1:B:418:LYS:O	2.36	0.44
1:B:734:ALA:HA	1:B:735:THR:HA	1.56	0.44
1:C:328:LEU:HB2	6:C:2517:HOH:O	2.17	0.44
1:C:577[B]:SER:HB2	6:C:2763:HOH:O	2.16	0.44
1:D:239:ASP:HB2	6:D:2317:HOH:O	2.17	0.44
1:A:22:THR:HG23	6:B:2996:HOH:O	2.17	0.44
1:A:51:HIS:CE1	1:A:52:CYS:O	2.71	0.44
1:B:132:THR:HB	1:B:137:VAL:HG23	2.00	0.44
1:C:260:SER:HB2	1:C:265:GLU:OE1	2.18	0.44
1:D:1019:LEU:N	1:D:1019:LEU:CD2	2.78	0.44
1:A:1007:ARG:CD	1:A:1011:TYR:HB2	2.47	0.44
1:A:644:SER:HA	1:A:671:CYS:SG	2.58	0.44
1:A:849:TRP:CH2	1:A:854:PRO:HG3	2.52	0.44
1:B:1007:ARG:CD	1:B:1011:TYR:HB2	2.47	0.44
1:B:300:ASP:HB3	6:B:2295:HOH:O	2.16	0.44
1:C:200:ILE:CD1	1:C:245[B]:ILE:HD11	2.47	0.44
1:C:459:TRP:HD1	6:C:2674:HOH:O	2.01	0.44
1:C:519:PRO:HB3	1:D:28:LEU:HD22	1.99	0.44
1:A:932:LEU:HD11	1:B:741:LEU:HD21	2.00	0.44
1:C:705:PRO:HA	1:C:730:ASP:OD2	2.17	0.44
1:C:779[B]:THR:HG23	1:C:929:LEU:CD2	2.47	0.44
1:D:57:ASN:HB2	6:D:2153:HOH:O	2.18	0.44
1:D:911:PRO:HG2	6:D:2470:HOH:O	2.17	0.44
1:A:705:PRO:HA	1:A:730:ASP:OD2	2.18	0.44
1:A:876:LEU:HD21	1:A:885:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:LYS:HE2	6:B:2291:HOH:O	2.17	0.44
1:D:394:ARG:C	1:D:395:LYS:HG3	2.38	0.44
1:A:868:ILE:HG22	1:A:870:GLU:H	1.83	0.44
1:B:360:PHE:HE2	6:B:2586:HOH:O	2.01	0.44
1:B:261:LEU:HD21	1:B:451:LEU:HD21	2.00	0.44
1:D:394:ARG:NH1	1:D:394:ARG:HG3	2.23	0.44
1:D:486:ALA:HA	6:D:2742:HOH:O	2.17	0.44
1:A:173:ASN:HD22	1:A:174:PRO:N	2.15	0.43
1:A:410:ARG:HG3	6:A:2603:HOH:O	2.17	0.43
1:C:200:ILE:HD13	1:C:245[B]:ILE:HD11	2.00	0.43
1:D:415:GLU:O	1:D:417:GLY:N	2.50	0.43
1:A:373:VAL:HG12	1:B:47:LYS:HD3	2.00	0.43
1:B:939:SER:OG	1:B:941:ILE:HG22	2.18	0.43
1:C:82:CYS:O	1:C:98:LYS:HD2	2.18	0.43
1:D:915:LYS:HG3	6:D:3141:HOH:O	2.17	0.43
1:A:223:VAL:CG2	1:A:245[A]:ILE:HD13	2.47	0.43
1:A:283:ILE:CG1	1:A:482:ILE:HD12	2.49	0.43
1:A:291:ASP:OD1	1:A:293:ILE:HG12	2.18	0.43
1:A:391:LEU:HD22	1:A:408:PHE:CG	2.53	0.43
1:A:859:HIS:HE1	6:A:3133:HOH:O	2.01	0.43
1:A:888:LYS:HD3	6:A:3027:HOH:O	2.17	0.43
1:B:100:PHE:C	1:B:100:PHE:CD1	2.92	0.43
1:D:358:ARG:NH2	6:D:2621:HOH:O	2.51	0.43
1:D:44:ASN:HB2	1:D:45:PRO:CD	2.47	0.43
1:B:934:THR:OG1	1:B:937:GLU:HG3	2.17	0.43
1:D:974:ASP:N	6:D:3200:HOH:O	2.51	0.43
1:B:643:CYS:HB2	1:B:650:TRP:CE2	2.53	0.43
1:B:863:LYS:HA	1:B:864:PRO:HD3	1.92	0.43
1:C:428:HIS:O	1:D:410:ARG:NH1	2.49	0.43
1:A:680:MET:HE1	6:A:2428:HOH:O	2.19	0.43
1:B:172:ARG:HG3	6:B:2329:HOH:O	2.17	0.43
1:B:378:GLU:HA	6:B:2627:HOH:O	2.19	0.43
1:A:132:THR:HB	1:A:137:VAL:HG23	2.00	0.43
1:C:423:GLU:OE1	1:C:423:GLU:HA	2.19	0.43
1:D:574:LYS:HB3	1:D:614:SER:HB2	2.01	0.43
1:A:311:PRO:O	1:A:315:LYS:HG3	2.19	0.43
1:D:859:HIS:CD2	1:D:862:GLY:H	2.20	0.43
1:A:25:HIS:CE1	6:B:2740:HOH:O	2.72	0.43
1:B:53:GLU:HB3	6:B:3072:HOH:O	2.17	0.43
1:C:1007:ARG:CD	1:C:1011:TYR:HB2	2.49	0.43
1:C:17:ALA:HB3	6:C:2038:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ARG:NH2	6:C:2548:HOH:O	2.52	0.43
1:D:391:LEU:HD22	1:D:408:PHE:CB	2.49	0.43
1:D:993:LEU:HD23	1:D:993:LEU:C	2.39	0.43
1:A:777:ALA:O	1:A:780:THR:HG22	2.19	0.42
1:A:932:LEU:HD21	6:B:2460:HOH:O	2.18	0.42
1:B:1007:ARG:HD3	1:B:1011:TYR:HB2	2.00	0.42
1:C:132:THR:HB	1:C:137:VAL:CG2	2.49	0.42
1:D:623:GLN:HG3	6:D:2880:HOH:O	2.18	0.42
1:A:67:LEU:HD23	1:B:146:GLU:HG2	2.00	0.42
1:C:993:LEU:C	1:C:993:LEU:HD23	2.40	0.42
1:D:672:PRO:HA	1:D:682:LEU:O	2.20	0.42
1:D:878:ASN:ND2	6:D:3117:HOH:O	2.52	0.42
1:C:54:LYS:HD3	1:C:891:ALA:HB1	2.01	0.42
1:C:391:LEU:CG	1:C:410[B]:ARG:HH12	2.31	0.42
1:C:828:GLN:HG3	6:C:2976:HOH:O	2.19	0.42
1:C:410[A]:ARG:HD3	1:C:422:ASP:OD2	2.20	0.42
1:A:397:ILE:CD1	1:A:428:HIS:HE1	2.31	0.42
1:C:323:ALA:O	1:C:324:CYS:C	2.58	0.42
1:C:572:LEU:HD13	1:C:638:ILE:HB	2.00	0.42
1:D:193:LEU:HD23	1:D:281:ILE:HD13	2.01	0.42
1:D:362:VAL:HG13	1:D:391:LEU:HD13	2.02	0.42
1:A:318:LYS:C	6:A:2503:HOH:O	2.58	0.42
1:B:621:TRP:O	1:B:625:VAL:HG23	2.19	0.42
1:C:423:GLU:OE1	1:C:423:GLU:CA	2.68	0.42
1:C:844:GLU:O	1:C:847:GLN:HG3	2.20	0.42
1:C:901:ASN:HD22	1:C:901:ASN:C	2.22	0.42
1:D:335:VAL:HG22	1:D:433:VAL:HB	2.02	0.42
1:D:910:LYS:HA	1:D:911:PRO:HD3	1.90	0.42
1:A:864:PRO:CD	6:A:3008:HOH:O	2.68	0.42
1:A:519:PRO:HB3	1:B:28:LEU:HD22	2.01	0.42
1:B:364:ARG:NH1	6:B:2639:HOH:O	2.53	0.42
1:A:32:LEU:HB2	1:B:485:MET:HE1	2.01	0.42
1:C:394:ARG:NH2	1:C:423:GLU:OE2	2.40	0.42
1:A:582:ILE:HD11	1:B:1015:ARG:CZ	2.50	0.42
1:B:1007:ARG:NH1	6:B:3174:HOH:O	2.51	0.42
1:B:364:ARG:HH11	1:B:364:ARG:HG3	1.85	0.42
1:B:36:LEU:HG	6:B:2098:HOH:O	2.19	0.42
1:B:381:LYS:HD3	6:B:2628:HOH:O	2.19	0.42
1:B:53:GLU:HB2	6:B:2150:HOH:O	2.20	0.42
1:C:577[A]:SER:HB3	6:C:2763:HOH:O	2.18	0.42
1:A:402:ARG:HH11	1:A:402:ARG:CG	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LYS:HG2	6:B:2386:HOH:O	2.20	0.42
1:B:263:GLU:HG2	1:B:449:GLU:OE1	2.20	0.42
1:C:19:ASN:OD1	1:C:20:PRO:HD2	2.20	0.42
1:A:870:GLU:O	1:A:889:ILE:HD13	2.20	0.41
1:A:893:GLU:OE2	1:A:896:ARG:CZ	2.68	0.41
1:B:611:GLU:O	5:B:1034:IUR:H6	2.20	0.41
1:C:28:LEU:HD22	1:D:519:PRO:HB3	2.02	0.41
1:C:346:ASP:OD2	4:C:1031:FAD:H6	2.20	0.41
1:C:409:VAL:N	1:C:410[B]:ARG:NH2	2.68	0.41
1:D:18:LEU:HD13	6:D:3199:HOH:O	2.19	0.41
1:D:934:THR:OG1	1:D:937:GLU:HG3	2.20	0.41
1:A:22:THR:CG2	6:B:2996:HOH:O	2.69	0.41
1:A:223:VAL:HG23	1:A:245[A]:ILE:HD13	2.03	0.41
1:A:191:ALA:HB2	1:A:276:TYR:CD2	2.56	0.41
1:B:1018:PRO:HA	6:B:3210:HOH:O	2.20	0.41
1:C:533:ILE:O	1:C:545:PRO:HD3	2.20	0.41
1:D:291:ASP:OD1	1:D:293:ILE:HG12	2.20	0.41
1:D:673:HIS:ND1	1:D:690:LEU:CD1	2.84	0.41
1:A:54:LYS:HG3	6:A:2120:HOH:O	2.21	0.41
1:A:673:HIS:C	1:A:673:HIS:ND1	2.70	0.41
1:A:989:CYS:O	1:A:990:THR:HB	2.20	0.41
1:D:140:CYS:HA	2:D:1027:SF4:S1	2.61	0.41
1:D:677:GLU:HG2	1:D:678:ARG:N	2.35	0.41
1:A:625:VAL:HG13	6:A:2822:HOH:O	2.20	0.41
1:B:273:GLU:HG3	6:B:2458:HOH:O	2.21	0.41
1:A:1017:LEU:HD12	1:B:620:TYR:N	2.35	0.41
1:A:555:THR:HA	1:A:574:LYS:HG3	2.01	0.41
1:B:237:PRO:HB2	1:B:239:ASP:OD1	2.20	0.41
1:B:391:LEU:HD23	1:B:408:PHE:HB3	2.02	0.41
1:B:52:CYS:HB2	1:B:384:LYS:CG	2.51	0.41
1:D:124:LEU:HD13	1:D:160:SER:HB2	2.03	0.41
1:A:1012:GLU:HA	1:A:1013:PRO:HD2	1.95	0.41
1:A:552:ALA:HB2	3:A:1030:FMN:HM73	2.03	0.41
1:A:691:VAL:HG21	1:A:720:ILE:HG23	2.03	0.41
1:A:993:LEU:HD23	1:A:993:LEU:C	2.41	0.41
1:B:291:ASP:OD1	1:B:293:ILE:HG12	2.21	0.41
1:A:100:PHE:CD1	1:A:100:PHE:C	2.93	0.41
1:B:828:GLN:NE2	6:B:2998:HOH:O	2.51	0.41
1:C:358:ARG:N	6:C:2549:HOH:O	2.54	0.41
6:C:2976:HOH:O	1:D:22:THR:CG2	2.69	0.41
1:A:193:LEU:HD23	1:A:281:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:HG3	6:A:2174:HOH:O	2.20	0.41
1:A:651:MET:HE3	1:A:700:GLN:HG3	2.01	0.41
1:B:27:ALA:HB2	6:B:2039:HOH:O	2.21	0.41
1:C:173:ASN:HA	1:C:174:PRO:HD3	1.90	0.41
1:C:413:GLN:HG2	1:C:417:GLY:O	2.19	0.41
1:D:237:PRO:HB2	1:D:239:ASP:OD1	2.20	0.41
1:D:705:PRO:HA	1:D:730:ASP:OD2	2.20	0.41
1:D:53:GLU:HG3	1:D:887:LYS:HD3	2.02	0.41
1:B:874:LYS:HE2	6:B:3057:HOH:O	2.21	0.41
1:C:315:LYS:NZ	6:C:2501:HOH:O	2.51	0.41
1:C:391:LEU:HD22	1:C:408:PHE:CG	2.56	0.41
1:A:371:ARG:HE	1:A:371:ARG:HB2	1.43	0.41
1:C:191:ALA:HB2	1:C:276:TYR:CD2	2.56	0.41
1:C:95:LEU:HD23	1:C:119:ASP:HB2	2.01	0.41
1:A:140:CYS:HA	2:A:1027:SF4:S1	2.61	0.40
1:A:259:LYS:NZ	6:A:2425:HOH:O	2.54	0.40
1:A:519:PRO:HD2	6:A:2707:HOH:O	2.20	0.40
1:A:621:TRP:O	1:A:625:VAL:HG23	2.21	0.40
1:B:629:LYS:CE	1:B:629:LYS:HA	2.51	0.40
1:C:323:ALA:HB1	1:C:904:PHE:CE2	2.56	0.40
1:D:311:PRO:O	1:D:315:LYS:CG	2.68	0.40
1:D:5:LEU:CD2	6:D:2001:HOH:O	2.64	0.40
1:D:883:LEU:HG	1:D:887:LYS:HE3	2.04	0.40
5:A:1034:IUR:I5	6:A:2798:HOH:O	2.93	0.40
1:B:863:LYS:NZ	6:B:3051:HOH:O	2.54	0.40
1:C:263:GLU:O	1:C:264:ASN:HB2	2.21	0.40
1:C:391:LEU:HD23	1:C:408:PHE:HB3	2.03	0.40
1:C:394:ARG:HG3	1:C:409:VAL:HG13	2.04	0.40
1:C:934:THR:OG1	1:C:937:GLU:HG3	2.21	0.40
1:D:391:LEU:CD2	1:D:408:PHE:CB	2.99	0.40
1:A:451:LEU:O	1:A:454:ILE:HG12	2.22	0.40
1:B:97:ILE:HD11	2:B:1026:SF4:S2	2.62	0.40
1:B:859:HIS:CD2	6:B:3039:HOH:O	2.74	0.40
1:C:223:VAL:HG23	6:C:2388:HOH:O	2.21	0.40
1:C:552:ALA:HB3	1:C:553:PRO:HD3	2.02	0.40
1:C:868:ILE:HG22	1:C:870:GLU:H	1.85	0.40
1:D:962[B]:THR:HG21	1:D:992:CYS:HA	2.03	0.40
1:A:97:ILE:HD11	2:A:1026:SF4:S2	2.61	0.40
1:A:173:ASN:HB2	6:A:2352:HOH:O	2.21	0.40
1:A:207:ALA:HB1	1:A:251:LEU:HB3	2.04	0.40
1:B:871:LEU:HB3	6:B:3054:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:LEU:CD2	1:C:408:PHE:HB2	2.52	0.40
1:C:518:LYS:O	1:C:520:GLU:HG3	2.21	0.40
1:D:231:ILE:HA	1:D:232:PRO:HD3	1.96	0.40
1:D:518:LYS:O	1:D:520:GLU:HG3	2.22	0.40
1:D:868:ILE:HG22	1:D:870:GLU:H	1.86	0.40
1:B:448:LYS:NZ	1:B:460:ASP:OD2	2.48	0.40
1:C:409:VAL:N	1:C:410[B]:ARG:HH21	2.20	0.40
1:C:501:TRP:CZ2	1:C:519:PRO:HA	2.57	0.40
1:D:97:ILE:HD11	2:D:1026:SF4:S2	2.61	0.40
1:D:367:PHE:CD1	1:D:370:ILE:HD11	2.57	0.40
1:D:83:ALA:O	1:D:84:ASP:C	2.60	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)
6:A:2001:HOH:O	6:A:2818:HOH:O[1_655]	1.98	0.22

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	1003/1025 (98%)	972 (97%)	29 (3%)	2 (0%)	51	28
1	B	1004/1025 (98%)	974 (97%)	29 (3%)	1 (0%)	55	32
1	C	1017/1025 (99%)	984 (97%)	30 (3%)	3 (0%)	44	23
1	D	1017/1025 (99%)	983 (97%)	31 (3%)	3 (0%)	44	23
All	All	4041/4100 (99%)	3913 (97%)	119 (3%)	9 (0%)	51	28

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	418	LYS
1	C	324	CYS
1	C	325	HIS
1	D	678	ARG
1	A	53	GLU
1	C	909	ARG
1	D	416	THR
1	D	415	GLU
1	A	416	THR

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	843/854 (99%)	831 (99%)	12 (1%)	71	50
1	B	845/854 (99%)	836 (99%)	9 (1%)	78	61
1	C	854/854 (100%)	842 (99%)	12 (1%)	71	50
1	D	852/854 (100%)	844 (99%)	8 (1%)	82	69
All	All	3394/3416 (99%)	3353 (99%)	41 (1%)	75	57

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	CYS
1	A	53	GLU
1	A	54	LYS
1	A	100	PHE
1	A	173	ASN
1	A	175	CYS
1	A	402	ARG
1	A	453	PRO
1	A	458	ARG
1	A	574	LYS
1	A	673	HIS
1	A	793	THR
1	B	100	PHE

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Mol	Chain	Res	Type
1	B	367	PHE
1	B	391	LEU
1	B	416	THR
1	B	453	PRO
1	B	574	LYS
1	B	793	THR
1	B	828	GLN
1	B	901	ASN
1	C	100	PHE
1	C	293	ILE
1	C	324	CYS
1	C	391	LEU
1	C	453	PRO
1	C	574	LYS
1	C	673	HIS
1	C	793	THR
1	C	828	GLN
1	C	857	GLU
1	C	901	ASN
1	C	907	LEU
1	D	100	PHE
1	D	367	PHE
1	D	453	PRO
1	D	673	HIS
1	D	793	THR
1	D	901	ASN
1	D	941	ILE
1	D	1019	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	295	GLN
1	A	407	GLN
1	A	428	HIS
1	A	703	GLN
1	A	828	GLN
1	A	859	HIS
1	A	885	GLN
1	B	295	GLN
1	B	407	GLN

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Mol	Chain	Res	Type
1	B	901	ASN
1	C	295	GLN
1	C	703	GLN
1	C	859	HIS
1	C	901	ASN
1	C	978	HIS
1	D	157	GLN
1	D	295	GLN
1	D	407	GLN
1	D	673	HIS
1	D	859	HIS
1	D	901	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

28 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	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1027	-	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	A	1028	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1029	-	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	A	1030	-	31,33,33	2.66	11 (35%)	38,50,50	3.15	12 (31%)
4	FAD	A	1031	-	51,58,58	2.15	20 (39%)	54,89,89	1.75	9 (16%)
5	IUR	A	1034	-	7,9,9	1.35	2 (28%)	6,12,12	11.15	4 (66%)
2	SF4	B	1026	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1027	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1028	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1029	-	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	B	1030	-	31,33,33	2.69	11 (35%)	38,50,50	3.16	13 (34%)
4	FAD	B	1031	-	51,58,58	2.14	19 (37%)	54,89,89	1.77	9 (16%)
5	IUR	B	1034	-	7,9,9	1.37	1 (14%)	6,12,12	11.22	4 (66%)
2	SF4	C	1026	-	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	-	31,33,33	2.73	11 (35%)	38,50,50	3.15	12 (31%)
4	FAD	C	1031	-	51,58,58	2.14	20 (39%)	54,89,89	1.76	8 (14%)
5	IUR	C	1034	-	7,9,9	1.50	1 (14%)	6,12,12	11.06	5 (83%)
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	-	31,33,33	2.72	11 (35%)	38,50,50	3.19	12 (31%)
4	FAD	D	1031	-	51,58,58	2.11	21 (41%)	54,89,89	1.75	9 (16%)
5	IUR	D	1034	-	7,9,9	1.40	1 (14%)	6,12,12	11.17	5 (83%)

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	-	-	0/0/48/48	2/6/5/5
2	SF4	A	1027	-	-	0/0/48/48	2/6/5/5
2	SF4	A	1028	-	-	0/0/48/48	2/6/5/5
2	SF4	A	1029	-	-	0/0/48/48	2/6/5/5
3	FMN	A	1030	-	-	0/16/18/18	0/3/3/3
4	FAD	A	1031	-	-	0/28/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IUR	A	1034	-	-	0/0/0/0	0/1/1/1
2	SF4	B	1026	-	-	0/0/48/48	2/6/5/5
2	SF4	B	1027	-	-	0/0/48/48	2/6/5/5
2	SF4	B	1028	-	-	0/0/48/48	2/6/5/5
2	SF4	B	1029	-	-	0/0/48/48	2/6/5/5
3	FMN	B	1030	-	-	0/16/18/18	0/3/3/3
4	FAD	B	1031	-	-	0/28/50/50	0/6/6/6
5	IUR	B	1034	-	-	0/0/0/0	0/1/1/1
2	SF4	C	1026	-	-	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	-	-	0/16/18/18	0/3/3/3
4	FAD	C	1031	-	-	0/28/50/50	0/6/6/6
5	IUR	C	1034	-	-	0/0/0/0	0/1/1/1
2	SF4	D	1026	1	-	0/0/48/48	2/6/5/5
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	-	-	0/16/18/18	0/3/3/3
4	FAD	D	1031	-	-	0/28/50/50	0/6/6/6
5	IUR	D	1034	-	-	0/0/0/0	0/1/1/1

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1030	FMN	C1'-N10	-9.33	1.38	1.48
3	D	1030	FMN	C1'-N10	-9.16	1.39	1.48
3	B	1030	FMN	C1'-N10	-9.13	1.39	1.48
3	A	1030	FMN	C1'-N10	-8.89	1.39	1.48
4	C	1031	FAD	PA-O2A	-3.83	1.35	1.55
4	A	1031	FAD	PA-O2A	-3.81	1.35	1.55
4	D	1031	FAD	PA-O2A	-3.80	1.36	1.55
4	B	1031	FAD	PA-O2A	-3.78	1.36	1.55
4	D	1031	FAD	P-O2P	-3.21	1.39	1.55
4	A	1031	FAD	P-O2P	-3.14	1.39	1.55
4	B	1031	FAD	P-O2P	-3.10	1.39	1.55
4	C	1031	FAD	P-O2P	-3.06	1.39	1.55
4	A	1031	FAD	C2B-C1B	-2.71	1.49	1.53
3	D	1030	FMN	C6-C5A	-2.69	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1030	FMN	C6-C5A	-2.53	1.38	1.41
4	A	1031	FAD	C2-N1	-2.44	1.33	1.38
4	D	1031	FAD	C2B-C1B	-2.40	1.49	1.53
3	C	1030	FMN	C6-C5A	-2.39	1.38	1.41
4	C	1031	FAD	C2-N1	-2.36	1.33	1.38
4	D	1031	FAD	C2-N1	-2.36	1.33	1.38
3	B	1030	FMN	C6-C5A	-2.34	1.38	1.41
4	C	1031	FAD	C2B-C1B	-2.34	1.49	1.53
4	B	1031	FAD	C2-N1	-2.29	1.33	1.38
4	B	1031	FAD	C2B-C1B	-2.20	1.50	1.53
5	A	1034	IUR	C6-N1	2.02	1.38	1.34
4	D	1031	FAD	C3B-C4B	2.03	1.58	1.53
3	C	1030	FMN	C4A-C10	2.04	1.44	1.41
4	C	1031	FAD	C5B-C4B	2.04	1.58	1.51
3	D	1030	FMN	C4A-C10	2.06	1.44	1.41
4	C	1031	FAD	O4B-C4B	2.08	1.49	1.45
3	B	1030	FMN	C4A-C10	2.08	1.44	1.41
4	A	1031	FAD	C5B-C4B	2.11	1.58	1.51
4	D	1031	FAD	C5B-C4B	2.11	1.58	1.51
4	B	1031	FAD	C2A-N1A	2.12	1.37	1.33
4	C	1031	FAD	C2A-N1A	2.15	1.37	1.33
4	C	1031	FAD	C5X-N5	2.19	1.38	1.35
3	A	1030	FMN	C4A-C10	2.21	1.44	1.41
4	D	1031	FAD	C2A-N1A	2.24	1.38	1.33
4	C	1031	FAD	C4A-N3A	2.25	1.38	1.35
4	A	1031	FAD	O4B-C4B	2.26	1.50	1.45
4	A	1031	FAD	C2A-N3A	2.29	1.36	1.32
4	C	1031	FAD	C2A-N3A	2.30	1.36	1.32
3	D	1030	FMN	C4-C4A	2.31	1.45	1.41
4	D	1031	FAD	O4B-C4B	2.31	1.50	1.45
4	D	1031	FAD	C5X-N5	2.31	1.38	1.35
4	A	1031	FAD	C2A-N1A	2.33	1.38	1.33
3	B	1030	FMN	C4-C4A	2.33	1.45	1.41
4	B	1031	FAD	O4B-C4B	2.40	1.50	1.45
4	D	1031	FAD	C4A-N3A	2.40	1.39	1.35
4	B	1031	FAD	C2A-N3A	2.45	1.36	1.32
4	A	1031	FAD	C5X-N5	2.45	1.39	1.35
4	B	1031	FAD	C4A-N3A	2.46	1.39	1.35
4	A	1031	FAD	C4A-N3A	2.47	1.39	1.35
4	C	1031	FAD	O5'-C5'	2.52	1.54	1.44
3	B	1030	FMN	C5A-N5	2.53	1.39	1.35
3	A	1030	FMN	C4-C4A	2.54	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1030	FMN	C4-C4A	2.57	1.46	1.41
4	B	1031	FAD	C5X-N5	2.57	1.39	1.35
4	A	1031	FAD	O5'-C5'	2.60	1.55	1.44
5	A	1034	IUR	C4-N3	2.63	1.37	1.33
3	D	1030	FMN	C4'-C3'	2.65	1.58	1.53
4	D	1031	FAD	O5'-C5'	2.65	1.55	1.44
4	D	1031	FAD	C2A-N3A	2.66	1.36	1.32
4	D	1031	FAD	C8-C7	2.67	1.47	1.41
4	B	1031	FAD	O5'-C5'	2.68	1.55	1.44
5	D	1034	IUR	C4-N3	2.71	1.38	1.33
3	D	1030	FMN	C5A-N5	2.73	1.39	1.35
4	D	1031	FAD	C4-C4X	2.75	1.46	1.41
3	A	1030	FMN	C4'-C3'	2.75	1.58	1.53
5	C	1034	IUR	C4-N3	2.75	1.38	1.33
4	C	1031	FAD	C4-C4X	2.76	1.46	1.41
3	C	1030	FMN	C4'-C3'	2.76	1.58	1.53
3	A	1030	FMN	C10-N1	2.78	1.37	1.33
3	D	1030	FMN	C10-N1	2.79	1.37	1.33
5	B	1034	IUR	C4-N3	2.79	1.38	1.33
4	C	1031	FAD	C8-C7	2.81	1.48	1.41
3	C	1030	FMN	C5A-N5	2.82	1.39	1.35
4	A	1031	FAD	C8-C7	2.83	1.48	1.41
3	C	1030	FMN	C10-N1	2.83	1.37	1.33
4	B	1031	FAD	C2-N3	2.84	1.43	1.38
4	B	1031	FAD	C8-C7	2.86	1.48	1.41
3	B	1030	FMN	C4'-C3'	2.86	1.59	1.53
4	D	1031	FAD	C10-N1	2.89	1.37	1.33
4	B	1031	FAD	C4-C4X	2.92	1.46	1.41
4	B	1031	FAD	C4X-N5	2.92	1.37	1.33
4	A	1031	FAD	C10-N1	2.95	1.37	1.33
4	C	1031	FAD	C2-N3	2.96	1.44	1.38
4	D	1031	FAD	C2-N3	2.96	1.44	1.38
4	A	1031	FAD	C4-C4X	2.97	1.47	1.41
4	A	1031	FAD	C4X-N5	2.97	1.37	1.33
3	B	1030	FMN	C10-N1	3.05	1.37	1.33
4	A	1031	FAD	C2-N3	3.12	1.44	1.38
4	C	1031	FAD	C10-N1	3.17	1.37	1.33
4	B	1031	FAD	C10-N1	3.19	1.37	1.33
3	A	1030	FMN	C5A-N5	3.22	1.40	1.35
4	C	1031	FAD	C4X-N5	3.24	1.38	1.33
4	D	1031	FAD	C4X-N5	3.31	1.38	1.33
4	D	1031	FAD	C4-N3	3.70	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1031	FAD	O4B-C1B	3.75	1.46	1.41
3	A	1030	FMN	C7M-C7	3.76	1.58	1.51
3	B	1030	FMN	C7M-C7	3.80	1.58	1.51
4	B	1031	FAD	O4B-C1B	3.80	1.46	1.41
3	D	1030	FMN	C7M-C7	3.93	1.58	1.51
4	B	1031	FAD	C4-N3	3.94	1.40	1.33
4	C	1031	FAD	C4-N3	3.96	1.40	1.33
4	D	1031	FAD	O4B-C1B	3.97	1.46	1.41
3	C	1030	FMN	C7M-C7	4.03	1.58	1.51
3	B	1030	FMN	C4-N3	4.08	1.40	1.33
4	C	1031	FAD	O4B-C1B	4.13	1.47	1.41
4	A	1031	FAD	C4-N3	4.13	1.40	1.33
3	D	1030	FMN	C4-N3	4.14	1.40	1.33
3	C	1030	FMN	C4-N3	4.16	1.40	1.33
3	A	1030	FMN	C4-N3	4.21	1.40	1.33
4	B	1031	FAD	C4X-C10	4.24	1.48	1.41
4	A	1031	FAD	C4X-C10	4.24	1.48	1.41
4	D	1031	FAD	C4X-C10	4.28	1.48	1.41
4	C	1031	FAD	C4X-C10	4.34	1.48	1.41
3	A	1030	FMN	C4A-N5	4.39	1.39	1.33
3	B	1030	FMN	C4A-N5	4.51	1.39	1.33
3	C	1030	FMN	C4A-N5	4.60	1.39	1.33
3	D	1030	FMN	C4A-N5	4.68	1.40	1.33
3	A	1030	FMN	C9A-N10	5.02	1.45	1.38
3	C	1030	FMN	C9A-N10	5.29	1.45	1.38
3	B	1030	FMN	C9A-N10	5.36	1.45	1.38
3	D	1030	FMN	C9A-N10	5.36	1.45	1.38
4	D	1031	FAD	C9A-N10	5.52	1.46	1.38
4	A	1031	FAD	C9A-N10	5.95	1.46	1.38
4	B	1031	FAD	C9A-N10	6.00	1.46	1.38
4	C	1031	FAD	C9A-N10	6.07	1.46	1.38

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1034	IUR	N1-C2-N3	-20.11	113.94	128.40
5	B	1034	IUR	N1-C2-N3	-19.94	114.06	128.40
5	C	1034	IUR	N1-C2-N3	-19.92	114.07	128.40
5	A	1034	IUR	N1-C2-N3	-19.78	114.17	128.40
3	D	1030	FMN	C4A-C4-N3	-7.77	112.42	123.48
5	B	1034	IUR	C5-C4-N3	-7.71	112.94	123.27
3	C	1030	FMN	C4A-C4-N3	-7.71	112.50	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1034	IUR	C5-C4-N3	-7.69	112.97	123.27
3	A	1030	FMN	C4A-C4-N3	-7.68	112.55	123.48
5	C	1034	IUR	C5-C4-N3	-7.67	113.00	123.27
5	D	1034	IUR	C5-C4-N3	-7.59	113.11	123.27
3	B	1030	FMN	C4A-C4-N3	-7.56	112.72	123.48
4	A	1031	FAD	C4X-C4-N3	-4.51	117.07	123.48
4	C	1031	FAD	C4X-C4-N3	-4.49	117.09	123.48
4	D	1031	FAD	C4X-C4-N3	-4.46	117.14	123.48
4	B	1031	FAD	C4X-C4-N3	-4.43	117.18	123.48
3	B	1030	FMN	O3'-C3'-C2'	-3.55	100.02	108.82
4	D	1031	FAD	N3A-C2A-N1A	-3.52	125.79	128.86
3	A	1030	FMN	O3'-C3'-C2'	-3.51	100.13	108.82
3	C	1030	FMN	O3'-C3'-C2'	-3.49	100.18	108.82
4	A	1031	FAD	N3A-C2A-N1A	-3.47	125.84	128.86
4	B	1031	FAD	N3A-C2A-N1A	-3.42	125.88	128.86
3	D	1030	FMN	O3'-C3'-C2'	-3.37	100.46	108.82
4	C	1031	FAD	N3A-C2A-N1A	-3.28	126.00	128.86
4	B	1031	FAD	C4-C4X-C10	-3.19	117.38	119.96
3	B	1030	FMN	C4-C4A-N5	-3.17	115.20	118.68
3	D	1030	FMN	C4-C4A-N5	-3.07	115.31	118.68
3	A	1030	FMN	C4-C4A-N5	-3.04	115.35	118.68
4	C	1031	FAD	C4-C4X-C10	-2.98	117.55	119.96
4	A	1031	FAD	C4-C4X-C10	-2.97	117.56	119.96
3	C	1030	FMN	C4-C4A-N5	-2.88	115.52	118.68
4	D	1031	FAD	C4-C4X-C10	-2.84	117.67	119.96
4	C	1031	FAD	C4X-C10-N10	-2.41	118.84	120.52
4	B	1031	FAD	C5X-C9A-N10	-2.38	115.89	117.66
4	A	1031	FAD	C5X-C9A-N10	-2.34	115.92	117.66
4	D	1031	FAD	C5X-C9A-N10	-2.31	115.94	117.66
4	C	1031	FAD	C5X-C9A-N10	-2.23	116.00	117.66
4	B	1031	FAD	C4X-C10-N10	-2.23	118.97	120.52
4	A	1031	FAD	C4X-C10-N10	-2.09	119.07	120.52
4	D	1031	FAD	C4X-C10-N10	-2.09	119.07	120.52
3	B	1030	FMN	C7-C6-C5A	-2.07	117.88	121.08
3	A	1030	FMN	C6-C5A-C9A	2.09	121.71	119.00
4	A	1031	FAD	C4A-C5A-N7A	2.14	111.48	109.41
3	C	1030	FMN	C6-C5A-C9A	2.15	121.79	119.00
5	D	1034	IUR	C6-C5-I5	2.15	122.05	118.79
5	C	1034	IUR	C6-C5-I5	2.16	122.06	118.79
4	B	1031	FAD	C4A-C5A-N7A	2.18	111.52	109.41
3	D	1030	FMN	C6-C5A-C9A	2.19	121.84	119.00
3	D	1030	FMN	O3'-C3'-C4'	2.19	114.25	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1031	FAD	C4A-C5A-N7A	2.23	111.57	109.41
3	C	1030	FMN	O3'-C3'-C4'	2.26	114.41	108.82
3	B	1030	FMN	C6-C5A-C9A	2.26	121.94	119.00
4	D	1031	FAD	C2A-N1A-C6A	2.29	122.77	118.77
4	C	1031	FAD	C2A-N1A-C6A	2.29	122.78	118.77
4	A	1031	FAD	C2A-N1A-C6A	2.31	122.81	118.77
3	B	1030	FMN	O3'-C3'-C4'	2.33	114.59	108.82
4	B	1031	FAD	C2A-N1A-C6A	2.39	122.96	118.77
3	A	1030	FMN	O3'-C3'-C4'	2.49	114.99	108.82
5	C	1034	IUR	C6-N1-C2	2.65	119.60	115.36
5	D	1034	IUR	C6-N1-C2	2.68	119.65	115.36
5	A	1034	IUR	C6-N1-C2	2.73	119.73	115.36
5	B	1034	IUR	C6-N1-C2	2.82	119.87	115.36
3	A	1030	FMN	C4A-N5-C5A	2.88	119.80	116.76
3	D	1030	FMN	P-O5'-C5'	3.12	126.88	118.30
3	B	1030	FMN	P-O5'-C5'	3.13	126.91	118.30
3	C	1030	FMN	C4A-N5-C5A	3.14	120.08	116.76
3	A	1030	FMN	P-O5'-C5'	3.15	126.98	118.30
3	C	1030	FMN	P-O5'-C5'	3.22	127.17	118.30
3	D	1030	FMN	C4A-N5-C5A	3.24	120.18	116.76
3	B	1030	FMN	C4A-N5-C5A	3.27	120.22	116.76
4	C	1031	FAD	O2A-PA-O1A	3.38	129.79	112.28
4	B	1031	FAD	O2A-PA-O1A	3.41	129.94	112.28
4	A	1031	FAD	O2A-PA-O1A	3.44	130.10	112.28
4	D	1031	FAD	O2A-PA-O1A	3.51	130.45	112.28
3	D	1030	FMN	O2'-C2'-C1'	3.59	118.09	109.79
3	C	1030	FMN	O2'-C2'-C1'	3.67	118.28	109.79
3	B	1030	FMN	O2'-C2'-C1'	3.68	118.30	109.79
3	C	1030	FMN	O4'-C4'-C3'	3.68	118.23	109.09
3	A	1030	FMN	O2'-C2'-C1'	3.69	118.31	109.79
3	A	1030	FMN	O4'-C4'-C3'	3.70	118.27	109.09
3	D	1030	FMN	O4'-C4'-C3'	3.73	118.35	109.09
3	B	1030	FMN	O4'-C4'-C3'	3.90	118.76	109.09
3	C	1030	FMN	C4-C4A-C10	4.41	123.53	119.96
3	A	1030	FMN	C4-C4A-C10	4.56	123.65	119.96
3	D	1030	FMN	C1'-N10-C9A	4.64	122.60	118.35
3	D	1030	FMN	C4-C4A-C10	4.67	123.74	119.96
3	A	1030	FMN	C1'-N10-C9A	4.69	122.65	118.35
3	B	1030	FMN	C1'-N10-C9A	4.69	122.65	118.35
3	B	1030	FMN	C4-C4A-C10	4.70	123.77	119.96
3	C	1030	FMN	C1'-N10-C9A	4.86	122.80	118.35
4	A	1031	FAD	C4-N3-C2	7.44	121.67	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1031	FAD	C4-N3-C2	7.56	121.77	115.16
4	C	1031	FAD	C4-N3-C2	7.74	121.93	115.16
4	B	1031	FAD	C4-N3-C2	7.76	121.94	115.16
3	B	1030	FMN	C4-N3-C2	13.19	126.70	115.16
3	A	1030	FMN	C4-N3-C2	13.22	126.72	115.16
3	C	1030	FMN	C4-N3-C2	13.23	126.73	115.16
3	D	1030	FMN	C4-N3-C2	13.49	126.95	115.16
5	C	1034	IUR	C4-N3-C2	16.32	129.43	115.16
5	D	1034	IUR	C4-N3-C2	16.56	129.64	115.16
5	A	1034	IUR	C4-N3-C2	16.83	129.88	115.16
5	B	1034	IUR	C4-N3-C2	16.91	129.95	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	A	1029	SF4	FE1-FE2-S3-S4
2	C	1029	SF4	FE1-FE2-S3-S4
2	B	1029	SF4	FE1-FE2-S3-S4
2	C	1027	SF4	FE3-FE4-S1-S2
2	D	1028	SF4	FE1-FE2-S3-S4
2	A	1027	SF4	FE3-FE4-S1-S2
2	B	1027	SF4	FE3-FE4-S1-S2
2	D	1027	SF4	FE3-FE4-S1-S2
2	C	1026	SF4	FE3-FE4-S1-S2
2	A	1026	SF4	FE1-FE2-S3-S4
2	C	1028	SF4	FE3-FE4-S1-S2
2	C	1028	SF4	FE1-FE2-S3-S4
2	B	1026	SF4	FE3-FE4-S1-S2
2	B	1028	SF4	FE1-FE2-S3-S4
2	D	1026	SF4	FE3-FE4-S1-S2
2	A	1028	SF4	FE3-FE4-S1-S2
2	B	1028	SF4	FE3-FE4-S1-S2
2	C	1027	SF4	FE1-FE2-S3-S4
2	A	1028	SF4	FE1-FE2-S3-S4
2	C	1026	SF4	FE1-FE2-S3-S4
2	D	1027	SF4	FE1-FE2-S3-S4
2	D	1028	SF4	FE3-FE4-S1-S2
2	A	1026	SF4	FE3-FE4-S1-S2

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Mol	Chain	Res	Type	Atoms
2	D	1026	SF4	FE1-FE2-S3-S4
2	A	1029	SF4	FE3-FE4-S1-S2
2	B	1026	SF4	FE1-FE2-S3-S4
2	A	1027	SF4	FE1-FE2-S3-S4
2	B	1027	SF4	FE1-FE2-S3-S4
2	B	1029	SF4	FE3-FE4-S1-S2
2	C	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	1026	SF4	1	0
2	A	1027	SF4	1	0
3	A	1030	FMN	1	0
4	A	1031	FAD	2	0
5	A	1034	IUR	1	0
2	B	1026	SF4	1	0
4	B	1031	FAD	2	0
5	B	1034	IUR	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1005/1025 (98%)	0.22	66 (6%) 19 18	11, 19, 38, 58	0
1	B	1005/1025 (98%)	0.22	77 (7%) 14 13	11, 19, 38, 58	0
1	C	1010/1025 (98%)	0.29	81 (8%) 13 12	11, 18, 40, 54	0
1	D	1014/1025 (98%)	0.28	88 (8%) 11 10	11, 18, 38, 55	0
All	All	4034/4100 (98%)	0.25	312 (7%) 14 13	11, 18, 39, 58	0

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	19.5
1	B	2	ALA	18.4
1	D	2	ALA	15.9
1	D	417	GLY	15.3
1	C	2	ALA	13.5
1	D	907	LEU	13.3
1	C	682	LEU	13.2
1	D	416	THR	12.9
1	A	324	CYS	12.8
1	D	676	GLY	12.6
1	C	416	THR	10.9
1	C	415	GLU	9.8
1	C	324	CYS	9.8
1	D	52	CYS	9.4
1	A	51	HIS	9.3
1	A	680	MET	9.3
1	C	675	MET	9.2
1	D	902	ALA	9.0
1	B	417	GLY	8.8
1	A	325	HIS	8.5
1	D	51	HIS	8.3

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Mol	Chain	Res	Type	RSRZ
1	B	867	ARG	8.3
1	B	1018	PRO	8.2
1	A	415	GLU	8.2
1	B	416	THR	8.1
1	A	682	LEU	7.8
1	A	417	GLY	7.8
1	B	901	ASN	7.8
1	C	325	HIS	7.7
1	D	901	ASN	7.6
1	A	867	ARG	7.6
1	D	459	TRP	7.5
1	B	367	PHE	7.2
1	C	872	MET	7.1
1	B	324	CYS	7.1
1	C	867	ARG	7.0
1	A	1017	LEU	7.0
1	A	416	THR	6.9
1	D	908	GLU	6.6
1	D	418	LYS	6.6
1	B	415	GLU	6.5
1	C	907	LEU	6.5
1	D	867	ARG	6.5
1	D	1019	LEU	6.5
1	C	51	HIS	6.5
1	D	675	MET	6.4
1	B	1017	LEU	6.4
1	A	175	CYS	6.4
1	A	50	PHE	6.4
1	B	673	HIS	6.3
1	A	52	CYS	6.3
1	B	682	LEU	6.2
1	B	680	MET	6.2
1	D	414	ASP	6.2
1	B	459	TRP	6.2
1	D	1010	PRO	6.1
1	C	459	TRP	6.1
1	C	322	CYS	6.1
1	A	901	ASN	6.1
1	C	1010	PRO	6.1
1	C	332	ARG	6.0
1	D	367	PHE	5.9
1	C	909	ARG	5.8

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Mol	Chain	Res	Type	RSRZ
1	D	872	MET	5.8
1	C	908	GLU	5.8
1	A	418	LYS	5.8
1	B	872	MET	5.7
1	B	52	CYS	5.7
1	B	418	LYS	5.6
1	B	900	GLN	5.6
1	A	908	GLU	5.6
1	C	52	CYS	5.5
1	D	175	CYS	5.4
1	D	900	GLN	5.4
1	A	673	HIS	5.4
1	B	908	GLU	5.3
1	B	51	HIS	5.2
1	C	901	ASN	5.2
1	B	899	GLU	5.2
1	C	673	HIS	5.2
1	C	423	GLU	5.2
1	B	869	ALA	5.1
1	C	418	LYS	5.0
1	C	367	PHE	5.0
1	B	458	ARG	4.9
1	C	391	LEU	4.9
1	C	674	GLY	4.9
1	D	899	GLU	4.9
1	C	323	ALA	4.8
1	B	410[A]	ARG	4.7
1	D	458	ARG	4.7
1	A	1010	PRO	4.7
1	D	869	ALA	4.7
1	D	673	HIS	4.7
1	D	677	GLU	4.6
1	B	175	CYS	4.6
1	C	910	LYS	4.6
1	C	417	GLY	4.6
1	A	322	CYS	4.5
1	C	320	GLY	4.5
1	A	391	LEU	4.4
1	D	1009	THR	4.4
1	B	180	GLU	4.4
1	C	419	TRP	4.3
1	C	904	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	414	ASP	4.3
1	B	1010	PRO	4.3
1	A	872	MET	4.3
1	C	326	SER	4.2
1	A	900	GLN	4.1
1	A	367	PHE	4.1
1	A	517	ALA	4.1
1	D	873	GLY	4.0
1	B	941	ILE	4.0
1	D	857	GLU	4.0
1	B	391	LEU	3.9
1	B	323	ALA	3.9
1	B	396	VAL	3.9
1	C	870	GLU	3.9
1	A	847	GLN	3.9
1	C	1017	LEU	3.8
1	A	870	GLU	3.8
1	D	420	ASN	3.8
1	C	869	ALA	3.8
1	C	330	SER	3.8
1	C	50	PHE	3.8
1	C	873	GLY	3.8
1	C	175	CYS	3.8
1	C	871	LEU	3.7
1	B	325	HIS	3.7
1	A	36	LEU	3.7
1	D	674	GLY	3.7
1	D	896	ARG	3.7
1	B	3	PRO	3.7
1	A	1009	THR	3.6
1	C	896	ARG	3.6
1	C	517	ALA	3.6
1	C	410[A]	ARG	3.6
1	C	1009	THR	3.6
1	A	896	ARG	3.6
1	D	419	TRP	3.6
1	C	414	ASP	3.5
1	A	3	PRO	3.5
1	D	1018	PRO	3.5
1	D	679	GLY	3.5
1	A	458	ARG	3.5
1	C	899	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	426	ILE	3.3
1	D	910	LYS	3.3
1	B	873	GLY	3.3
1	A	910	LYS	3.3
1	C	900	GLN	3.2
1	B	414	ASP	3.2
1	A	181	LYS	3.2
1	A	332	ARG	3.2
1	B	896	ARG	3.2
1	A	426	ILE	3.2
1	A	873	GLY	3.2
1	A	49	CYS	3.1
1	D	322	CYS	3.1
1	D	391	LEU	3.1
1	D	682	LEU	3.1
1	A	696	ARG	3.1
1	B	332	ARG	3.1
1	D	295	GLN	3.1
1	B	518	LYS	3.0
1	D	180	GLU	3.0
1	D	941	ILE	3.0
1	A	1012	GLU	3.0
1	A	681	GLY	3.0
1	C	331	ILE	3.0
1	A	869	ALA	3.0
1	D	689	GLU	3.0
1	D	371	ARG	2.9
1	A	22	THR	2.9
1	C	903	ALA	2.9
1	D	3	PRO	2.9
1	B	1008	THR	2.9
1	C	902	ALA	2.9
1	B	870	GLU	2.9
1	D	856	THR	2.9
1	A	518	LYS	2.8
1	A	941	ILE	2.8
1	C	420	ASN	2.8
1	D	53	GLU	2.8
1	D	415	GLU	2.8
1	B	295	GLN	2.8
1	A	319	ALA	2.8
1	A	899	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	420	ASN	2.8
1	B	443	ARG	2.7
1	C	49	CYS	2.7
1	B	424	ASP	2.7
1	A	1008	THR	2.7
1	D	1012	GLU	2.7
1	D	332	ARG	2.7
1	C	917	PRO	2.7
1	C	1012	GLU	2.7
1	D	22	THR	2.7
1	D	181	LYS	2.7
1	C	53	GLU	2.7
1	C	3	PRO	2.7
1	C	329	PRO	2.7
1	B	36	LEU	2.7
1	C	847	GLN	2.7
1	A	323	ALA	2.6
1	B	910	LYS	2.6
1	A	897	LEU	2.6
1	D	413	GLN	2.6
1	B	517	ALA	2.6
1	B	847	GLN	2.6
1	A	459	TRP	2.6
1	D	678	ARG	2.6
1	B	319	ALA	2.6
1	B	50	PHE	2.6
1	C	1008	THR	2.6
1	B	328	LEU	2.6
1	B	519	PRO	2.6
1	C	906	PRO	2.6
1	D	179	GLN	2.6
1	A	273	GLU	2.5
1	D	300	ASP	2.5
1	B	402	ARG	2.5
1	D	325	HIS	2.5
1	C	458	ARG	2.5
1	B	672	PRO	2.5
1	B	856	THR	2.5
1	D	847	GLN	2.5
1	D	49	CYS	2.5
1	B	419	TRP	2.5
1	C	868	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	10	ALA	2.5
1	B	54	LYS	2.5
1	D	36	LEU	2.5
1	A	1016	GLY	2.5
1	C	413	GLN	2.5
1	C	319	ALA	2.4
1	C	273	GLU	2.4
1	B	700	GLN	2.4
1	B	681	GLY	2.4
1	B	420	ASN	2.4
1	C	913	ILE	2.4
1	D	913	ILE	2.4
1	D	50	PHE	2.4
1	D	680	MET	2.4
1	D	402	ARG	2.4
1	A	180	GLU	2.4
1	A	913	ILE	2.4
1	C	672	PRO	2.4
1	A	1011	TYR	2.4
1	B	364	ARG	2.4
1	D	485	MET	2.4
1	D	871	LEU	2.3
1	B	11	ASP	2.3
1	C	696	ARG	2.3
1	D	1017	LEU	2.3
1	B	320	GLY	2.3
1	B	520	GLU	2.3
1	B	857	GLU	2.3
1	D	423	GLU	2.3
1	B	296	GLY	2.3
1	D	1011	TYR	2.3
1	D	909	ARG	2.3
1	D	874	LYS	2.3
1	D	898	LYS	2.3
1	B	1011	TYR	2.3
1	C	1011	TYR	2.3
1	A	857	GLU	2.2
1	A	178	SER	2.2
1	C	916	LYS	2.2
1	D	844	GLU	2.2
1	D	915	LYS	2.2
1	D	870	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	273	GLU	2.2
1	A	419	TRP	2.2
1	B	703	GLN	2.2
1	B	387	PHE	2.2
1	C	857	GLU	2.2
1	B	179	GLN	2.2
1	D	866	PRO	2.2
1	A	868	ILE	2.2
1	C	424	ASP	2.2
1	D	54	LYS	2.2
1	B	407	GLN	2.1
1	C	371	ARG	2.1
1	D	364	ARG	2.1
1	D	696	ARG	2.1
1	A	424	ASP	2.1
1	D	424	ASP	2.1
1	C	402	ARG	2.1
1	B	1012	GLU	2.1
1	D	517	ALA	2.1
1	D	487	ASN	2.1
1	B	181	LYS	2.1
1	C	874	LYS	2.1
1	C	180	GLU	2.1
1	D	289	LYS	2.1
1	B	371	ARG	2.1
1	C	915	LYS	2.1
1	A	402	ARG	2.1
1	B	917	PRO	2.1
1	C	357	ARG	2.1
1	D	868	ILE	2.1
1	C	518	LYS	2.1
1	D	443	ARG	2.1
1	A	885	GLN	2.0
1	B	395	LYS	2.0
1	D	917	PRO	2.0
1	D	916	LYS	2.0
1	B	22	THR	2.0
1	A	23	GLN	2.0
1	B	176	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	IUR	A	1034	9/9	0.98	0.10	1.04	18,19,22,29	0
5	IUR	B	1034	9/9	0.98	0.09	0.19	18,19,21,30	0
5	IUR	C	1034	9/9	0.98	0.09	0.16	17,18,20,25	0
2	SF4	A	1028	8/8	0.97	0.07	0.05	14,15,16,17	0
4	FAD	A	1031	53/53	0.96	0.10	-0.04	13,14,16,17	0
2	SF4	B	1029	8/8	0.97	0.08	-0.07	14,15,17,17	0
4	FAD	B	1031	53/53	0.97	0.08	-0.22	13,15,17,18	0
3	FMN	A	1030	31/31	0.96	0.07	-0.26	13,14,16,18	0
2	SF4	B	1026	8/8	0.97	0.07	-0.29	13,13,15,16	0
3	FMN	D	1030	31/31	0.97	0.08	-0.30	11,13,14,15	0
2	SF4	A	1029	8/8	0.96	0.08	-0.33	15,16,18,18	0
2	SF4	A	1026	8/8	0.97	0.07	-0.40	12,13,15,16	0
2	SF4	C	1027	8/8	0.97	0.08	-0.44	12,12,14,15	0
4	FAD	D	1031	53/53	0.97	0.08	-0.45	13,15,16,18	0
5	IUR	D	1034	9/9	0.99	0.08	-0.46	15,16,19,25	0
2	SF4	A	1027	8/8	0.98	0.07	-0.49	12,12,14,15	0
3	FMN	C	1030	31/31	0.97	0.07	-0.55	11,14,15,15	0
4	FAD	C	1031	53/53	0.96	0.07	-0.58	14,15,17,18	0
2	SF4	B	1028	8/8	0.97	0.07	-0.64	14,14,16,17	0
2	SF4	D	1029	8/8	0.97	0.07	-0.65	14,14,16,17	0
2	SF4	C	1026	8/8	0.97	0.07	-0.74	12,14,15,15	0
2	SF4	D	1027	8/8	0.97	0.07	-0.76	11,11,14,14	0
2	SF4	D	1026	8/8	0.97	0.07	-0.78	12,13,15,15	0
2	SF4	D	1028	8/8	0.98	0.07	-0.79	13,14,16,17	0
3	FMN	B	1030	31/31	0.97	0.06	-0.86	13,15,17,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SF4	B	1027	8/8	0.98	0.07	-0.96	12,12,15,15	0
2	SF4	C	1028	8/8	0.98	0.07	-0.96	13,13,15,16	0
2	SF4	C	1029	8/8	0.97	0.07	-1.06	12,13,15,15	0

6.5 Other polymers

There are no such residues in this entry.