

Full wwPDB X-ray Structure Validation Report (i)

Oct 14, 2023 – 04:22 PM EDT

PDB ID	:	8F61
Title	:	Dihydropyrimidine Dehydrogenase (DPD) C671S Mutant Soaked with Dihy-
		drothymine Quasi-Anaerobically
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Deposited on	:	2022-11-15
Resolution	:	2.14 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.14 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	А	1025	83%	16%	••
1	В	1025	4%	15%	••
1	С	1025	4% 82%	16%	
1	D	1025	4%	17%	•

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	В	1102	-	-	Х	-



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 32219 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	Δ	1016	Total	С	Ν	Ο	\mathbf{S}	66	0	0	
	A	1010	7721	4897	1303	1466	55	00	0	0	
1	р	1016	Total	С	Ν	Ο	S	70	0	0	
	1010	7740	4910	1311	1464	55	10	0	U		
1	C	1010	Total	С	Ν	Ο	S	66	0	0	
	1010	7721	4897	1303	1466	55	00	0	0		
1 D	1016	Total	С	Ν	Ο	S	70	0	0		
	1010	7740	4910	1311	1464	55		0			

• Molecule 1 is a protein called Dihydropyrimidine dehydrogenase [NADP(+)].

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	60	ASP	GLY	conflict	UNP Q28943
А	671	SER	CYS	engineered mutation	UNP Q28943
В	60	ASP	GLY	conflict	UNP Q28943
В	671	SER	CYS	engineered mutation	UNP Q28943
С	60	ASP	GLY	conflict	UNP Q28943
С	671	SER	CYS	engineered mutation	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943
D	671	SER	CYS	engineered mutation	UNP Q28943

• Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	TotalFeS844	0	0
2	А	1	Total Fe S 8 4 4	0	0
2	А	1	TotalFeS844	0	0
2	А	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	С	1	TotalFeS844	0	0
2	С	1	TotalFeS844	0	0
2	С	1	TotalFeS844	0	0
2	С	1	TotalFeS844	0	0
2	D	1	TotalFeS844	0	0
2	D	1	Total Fe S 8 4 4	0	0



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

• Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	
3	Λ	1	Total	С	Ν	Ο	Р	0	0
5	Л	1	53	27	9	15	2	0	0
3	D	1	Total	С	Ν	Ο	Р	0	0
J D	D	1	53	27	9	15	2	0	0
2	С	1	Total	С	Ν	0	Р	0	0
5	U	1	53	27	9	15	2	0	0
2	Л	D 1	Total	С	Ν	Ο	Р	0	0
3	D		53	27	9	15	2	0	0

• Molecule 4 is THYMINE (three-letter code: TDR) (formula: C₅H₆N₂O₂) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Ato	ms		ZeroOcc	AltConf
4	А	1	Total C 9 5	N 2	O 2	0	0
4	D	1	Total C 9 5	N 2	O 2	0	0

• Molecule 5 is 1-DEOXY-1-(7,8-DIMETHYL-2,4-DIOXO-3,4-DIHYDRO-2H-BENZO[G]P TERIDIN-1-ID-10(5H)-YL)-5-O-PHOSPHONATO-D-RIBITOL (three-letter code: FNR) (formula: C₁₇H₂₃N₄O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
5	Δ	1	Total	С	Ν	0	Р	0	0
5	A	1	31	17	4	9	1	0	U



Mol	Chain	Residues		Ato	\mathbf{pms}			ZeroOcc	AltConf
Б.	Л	1	Total	С	Ν	0	Р	0	0
0	D	1	31	17	4	9	1	0	0

• Molecule 6 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
6	р	1	Total	С	Ν	Ο	Р	0	0
0 В	1	31	17	4	9	1	0	0	
6	C	1	Total	С	Ν	0	Р	0	0
0		L	31	17	4	9	1	0	0

• Molecule 7 is (5S)-5-methyl-1,3-diazinane-2,4-dione (three-letter code: XH5) (formula: $C_5H_8N_2O_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	В	1	Total 9	С 5	N 2	O 2	0	0
7	С	1	Total 9	С 5	N 2	O 2	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	187	Total O 187 187	0	0
8	В	208	Total O 208 208	0	0
8	С	198	Total O 198 198	0	0
8	D	204	Total O 204 204	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 [NADP(+)]











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	81.78Å 157.67Å 162.56Å	Depositor
a, b, c, α , β , γ	90.00° 95.93° 90.00°	Depositor
Bosolution(A)	161.69 - 2.14	Depositor
Resolution (A)	161.69 - 2.14	EDS
% Data completeness	52.7(161.69-2.14)	Depositor
(in resolution range)	52.7 (161.69-2.14)	EDS
R_{merge}	0.17	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.58 (at 2.14 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.187 , 0.230	Depositor
n, n_{free}	0.187 , 0.229	DCC
R_{free} test set	5647 reflections (4.78%)	wwPDB-VP
Wilson B-factor $(Å^2)$	26.0	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.38 , 51.7	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32219	wwPDB-VP
Average B, all atoms $(Å^2)$	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: TDR, FNR, FMN, XH5, FAD, SF4

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ # Z > 5		RMSZ	# Z > 5	
1	А	0.27	0/7881	0.50	0/10684	
1	В	0.27	0/7902	0.51	0/10710	
1	С	0.27	0/7881	0.50	0/10684	
1	D	0.28	0/7902	0.51	0/10710	
All	All	0.27	0/31566	0.51	0/42788	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	А	7721	0	7726	111	0
1	В	7740	0	7763	100	0
1	С	7721	0	7726	93	0
1	D	7740	0	7763	108	0
2	А	32	0	0	0	0
2	В	32	0	0	2	0
2	С	32	0	0	0	0
2	D	32	0	0	1	0
3	А	53	0	31	1	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	53	0	31	3	0
3	С	53	0	31	3	0
3	D	53	0	31	2	0
4	А	9	0	6	1	0
4	D	9	0	6	0	0
5	А	31	0	21	3	0
5	D	31	0	21	2	0
6	В	31	0	19	0	0
6	С	31	0	19	0	0
7	В	9	0	0	0	0
7	С	9	0	0	0	0
8	А	187	0	0	16	0
8	В	208	0	0	12	1
8	С	198	0	0	10	0
8	D	204	0	0	17	1
All	All	32219	0	31194	383	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 6.

All (383) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:38:LYS:NZ	8:C:1202:HOH:O	1.98	0.97
1:C:372:ALA:O	8:C:1201:HOH:O	1.88	0.90
1:A:297:LEU:HD11	1:A:396:VAL:HG11	1.60	0.84
1:A:463:GLU:O	8:A:1201:HOH:O	1.98	0.81
1:D:219:LYS:HG3	1:D:260:SER:HB2	1.64	0.80
1:B:364:ARG:NH1	8:B:1205:HOH:O	2.15	0.79
1:C:672:PRO:O	8:C:1203:HOH:O	1.99	0.79
1:A:913:ILE:O	8:A:1202:HOH:O	2.01	0.78
1:A:364:ARG:H	1:A:364:ARG:HD3	1.47	0.78
1:D:481:ASP:OD2	8:D:1201:HOH:O	2.01	0.77
1:A:52:CYS:HB3	1:A:384:LYS:HB2	1.67	0.77
1:A:651:MET:HG2	1:A:701:ALA:HB2	1.65	0.76
1:A:80:LEU:O	8:A:1204:HOH:O	2.04	0.76
1:A:442:LEU:HD22	1:A:482:ILE:HD11	1.70	0.73
1:D:134:ASP:OD1	8:D:1202:HOH:O	2.06	0.73
1:B:178:SER:HB3	1:B:181:LYS:HE2	1.70	0.72
3:C:1105:FAD:O2A	8:C:1204:HOH:O	2.07	0.71
1:C:124:LEU:HD13	1:C:160:SER:HB2	1.72	0.71



	A + O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:950:GLU:HG2	1:B:979:LEU:HD22	1.72	0.71
1:D:910:LYS:HD3	1:D:911:PRO:HD2	1.73	0.71
1:B:106:ASN:O	8:B:1201:HOH:O	2.08	0.71
1:A:23:GLN:NE2	1:B:96:ASP:OD2	2.23	0.70
1:C:857:GLU:OE2	1:C:867:ARG:NH2	2.25	0.70
1:D:230:GLU:OE1	8:D:1203:HOH:O	2.10	0.70
1:A:909:ARG:O	8:A:1205:HOH:O	2.09	0.69
1:D:927:LYS:NZ	8:D:1216:HOH:O	2.25	0.69
1:B:298:THR:H	1:B:301:GLN:HE21	1.40	0.69
1:A:761:THR:O	8:A:1206:HOH:O	2.11	0.68
1:D:650:TRP:O	1:D:654:SER:OG	2.11	0.68
1:D:764:GLY:O	8:D:1204:HOH:O	2.11	0.68
1:D:328:LEU:HD12	1:D:329:PRO:HD2	1.74	0.67
1:B:269:ASN:ND2	8:B:1214:HOH:O	2.28	0.67
1:A:1007:ARG:HD3	1:A:1011:TYR:HB2	1.77	0.67
1:C:783:ARG:HG3	1:C:929:LEU:HD22	1.76	0.67
1:B:130:CYS:CB	2:B:1102:SF4:S4	2.78	0.67
1:C:343:THR:HA	3:C:1105:FAD:HM73	1.77	0.67
1:A:800:GLU:O	8:A:1208:HOH:O	2.13	0.66
1:A:466:PRO:O	8:A:1207:HOH:O	2.13	0.66
1:B:5:LEU:O	8:B:1202:HOH:O	2.12	0.66
1:D:651:MET:HG2	1:D:701:ALA:HB2	1.78	0.65
1:D:680:MET:O	1:D:680:MET:HG3	1.97	0.65
1:D:685:GLY:O	8:D:1205:HOH:O	2.14	0.65
1:B:730:ASP:O	8:B:1204:HOH:O	2.14	0.64
1:C:374:PRO:HA	1:C:377:VAL:HG12	1.80	0.63
1:B:697:TRP:O	1:B:700:GLN:HB2	1.99	0.63
1:C:23:GLN:NE2	1:D:96:ASP:OD2	2.31	0.62
1:C:335:VAL:HG22	1:C:433:VAL:HB	1.81	0.61
1:D:581:ASP:OD2	8:D:1209:HOH:O	2.16	0.61
1:B:584:THR:O	8:B:1206:HOH:O	2.17	0.60
1:B:699:ARG:HE	1:B:699:ARG:HA	1.65	0.60
1:C:647:LYS:O	1:C:651:MET:HG3	2.01	0.60
1:D:106:ASN:O	8:D:1206:HOH:O	2.16	0.59
1:C:42:LYS:NZ	8:D:1202:HOH:O	2.24	0.59
1:D:673:HIS:HB2	8:D:1208:HOH:O	2.02	0.59
1:D:948:ILE:HG12	1:D:1002:ILE:HG12	1.83	0.59
1:B:399:LYS:HG3	1:B:404:VAL:HG21	1.85	0.59
1:A:741:LEU:HD11	1:B:932:LEU:HD11	1.85	0.59
1:B:362:VAL:HG22	1:B:388:LEU:HB2	1.84	0.59
1:C:329:PRO:HB2	1:C:331:ILE:HD13	1.85	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:367:PHE:HA	1:D:370:ILE:HD11	1.84	0.59
1:B:725:LYS:HD3	1:B:785:LEU:HD22	1.85	0.59
1:A:738:VAL:HG11	1:B:773:ILE:HD11	1.84	0.58
1:C:242:ASN:ND2	8:C:1215:HOH:O	2.35	0.58
1:A:57:ASN:O	1:A:57:ASN:ND2	2.37	0.58
1:B:783:ARG:HG2	1:B:929:LEU:HD22	1.85	0.58
1:A:793:THR:HG22	1:A:814:GLN:HB2	1.84	0.57
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.87	0.57
1:A:491:GLU:OE2	1:B:35:LYS:NZ	2.37	0.57
1:C:740:GLY:HA2	1:D:776:ARG:HB2	1.86	0.57
1:B:63:LYS:HE3	1:B:128:MET:HG2	1.87	0.56
1:C:675:MET:SD	1:C:675:MET:N	2.78	0.56
1:D:242:ASN:O	1:D:246:GLU:HG2	2.05	0.56
1:D:367:PHE:HZ	1:D:387:PHE:HB2	1.70	0.56
1:A:337:VAL:HB	1:A:361:LEU:HD13	1.88	0.56
1:B:298:THR:H	1:B:301:GLN:NE2	2.03	0.56
1:D:574:LYS:NZ	5:D:1107:FNR:O4	2.34	0.56
1:D:834:LEU:HD21	1:D:921:ILE:HD11	1.87	0.56
1:B:886:ARG:O	1:B:890:ILE:HG13	2.06	0.56
1:C:948:ILE:HD13	1:C:980:PRO:HG2	1.86	0.56
1:A:399:LYS:HB2	1:A:404:VAL:HG21	1.88	0.56
1:A:859:HIS:NE2	8:A:1217:HOH:O	2.31	0.56
1:A:343:THR:HA	3:A:1105:FAD:HM73	1.88	0.56
1:D:423:GLU:OE2	1:D:423:GLU:N	2.39	0.56
1:D:330:SER:OG	1:D:330:SER:O	2.24	0.55
1:D:370:ILE:HD12	1:D:370:ILE:H	1.70	0.55
1:D:889:ILE:HD12	1:D:889:ILE:H	1.71	0.55
1:B:541:LYS:NZ	8:B:1227:HOH:O	2.39	0.55
1:C:193:LEU:HD23	1:C:281:ILE:HD13	1.87	0.55
1:D:63:LYS:HE3	1:D:128:MET:HG2	1.89	0.55
1:A:532:ASP:O	8:A:1209:HOH:O	2.18	0.55
1:C:140:CYS:HB3	1:C:149:SER:HB3	1.88	0.55
1:C:1007:ARG:HD3	1:C:1011:TYR:HB2	1.89	0.55
1:C:673:HIS:HB2	8:C:1203:HOH:O	2.07	0.54
1:A:245:ILE:HG22	1:A:249:LYS:HD2	1.88	0.54
1:A:950:GLU:HG2	1:A:979:LEU:HD22	1.90	0.54
1:C:779:THR:HG21	1:C:932:LEU:HG	1.89	0.54
1:B:95:LEU:HD21	1:B:116:ILE:HG23	1.90	0.54
1:C:294:PHE:HA	1:C:297:LEU:HD12	1.90	0.53
1:C:162:VAL:O	1:C:166:MET:HG3	2.08	0.53
1:D:88:GLN:NE2	8:D:1217:HOH:O	2.25	0.53



		Interatomic Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:318:LYS:NZ	8:C:1212:HOH:O	2.29	0.53
1:D:180:GLU:CD	1:D:180:GLU:H	2.11	0.53
1:C:882:TYR:O	1:C:886:ARG:HG3	2.09	0.53
1:B:789:PRO:HG2	8:B:1204:HOH:O	2.07	0.53
1:C:901:ASN:O	1:C:901:ASN:ND2	2.42	0.53
1:C:192:LEU:HG	1:C:280:PHE:HB3	1.92	0.52
1:D:343:THR:HA	3:D:1105:FAD:HM73	1.92	0.52
1:B:845:GLU:N	1:B:845:GLU:OE1	2.42	0.52
1:C:18:LEU:HD11	1:C:975:PRO:HA	1.92	0.52
1:C:63:LYS:HE3	1:C:128:MET:HG2	1.90	0.52
1:C:373:VAL:HG22	1:C:375:GLU:HG3	1.92	0.52
1:D:710:LEU:HD22	1:D:720:ILE:HG22	1.91	0.52
1:D:95:LEU:HD11	1:D:120:ASN:HB2	1.92	0.52
1:C:598:PRO:HG3	1:D:107:LYS:HE3	1.91	0.51
1:B:346:ASP:OD2	3:B:1105:FAD:H6	2.11	0.51
1:D:381:LYS:HD2	1:D:381:LYS:C	2.30	0.51
1:D:893:GLU:OE1	8:D:1210:HOH:O	2.18	0.51
1:A:288:PRO:HG3	1:A:307:LYS:HB2	1.92	0.51
1:B:466:PRO:O	8:B:1207:HOH:O	2.19	0.51
1:C:167:ASN:ND2	1:C:910:LYS:O	2.43	0.51
1:A:32:LEU:HD13	1:A:36:LEU:HD11	1.92	0.51
1:B:796:ILE:HD13	1:B:813:LEU:HB3	1.93	0.51
1:B:844:GLU:O	1:B:847:GLN:HG3	2.11	0.51
1:D:889:ILE:HD12	1:D:889:ILE:N	2.26	0.51
1:A:261:LEU:HD21	1:A:451:LEU:HD21	1.93	0.51
1:A:50:PHE:HA	1:B:368:VAL:HG12	1.93	0.51
1:C:345:PHE:HE1	1:C:387:PHE:HE2	1.56	0.51
1:D:457:ASN:HB3	1:D:463:GLU:HG3	1.92	0.51
1:A:28:LEU:HD21	1:B:521:LEU:HG	1.91	0.51
1:A:54:LYS:HE3	1:A:895:MET:HG2	1.94	0.50
1:D:86:PRO:HA	1:D:89:LYS:HG3	1.93	0.50
1:A:18:LEU:HD11	1:A:975:PRO:HA	1.93	0.50
1:B:574:LYS:HB3	1:B:614:SER:HB2	1.94	0.50
1:C:366:GLY:H	1:C:369:ASN:HD22	1.59	0.50
1:D:97:ILE:HD11	2:D:1102:SF4:S1	2.52	0.49
1:B:208:ARG:HB3	1:B:522:PRO:HG2	1.94	0.49
1:A:552:ALA:HB2	5:A:1107:FNR:H7M3	1.95	0.49
1:A:131:PRO:HB2	1:A:373:VAL:HG11	1.93	0.49
1:C:23:GLN:NE2	8:C:1233:HOH:O	2.44	0.49
1:A:929:LEU:HB2	1:C:941:ILE:HG13	1.95	0.49
1:D:669:LEU:HD11	1:D:708:ALA:HB1	1.94	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:95:LEU:HD23	1:A:119:ASP:HB2	1.94	0.49
1:D:272:LYS:HG2	1:D:475:TRP:CZ2	2.48	0.49
1:C:793:THR:HB	1:C:814:GLN:HB2	1.95	0.49
1:D:451:LEU:O	1:D:454:ILE:HG12	2.12	0.49
1:B:699:ARG:NH2	1:B:704:ILE:O	2.46	0.49
1:A:557:SER:HB2	1:A:628:LEU:HD11	1.95	0.48
1:C:267:THR:OG1	1:C:270:THR:HG23	2.13	0.48
1:A:348:ALA:CB	1:A:361:LEU:HD21	2.42	0.48
1:A:672:PRO:HA	1:A:683:ALA:HA	1.96	0.48
1:D:340:ALA:HB1	1:D:370:ILE:HG23	1.95	0.48
1:A:520:GLU:HB3	1:B:25:HIS:CD2	2.48	0.48
1:B:908:GLU:O	1:B:910:LYS:N	2.47	0.48
1:C:709:LYS:HA	1:C:733:THR:HB	1.95	0.48
1:C:866:PRO:HG2	1:C:890:ILE:HD13	1.95	0.48
1:A:574:LYS:NZ	5:A:1107:FNR:H5	2.10	0.48
1:A:940:ASN:HA	8:A:1215:HOH:O	2.13	0.48
1:B:171:ILE:HG23	1:B:527:PRO:HD3	1.94	0.48
1:D:346:ASP:OD2	3:D:1105:FAD:H6	2.13	0.48
1:D:923:ASP:O	1:D:927:LYS:HE2	2.14	0.48
1:D:859:HIS:H	1:D:952:MET:HG2	1.79	0.48
1:B:291:ASP:OD1	1:B:292:ASP:N	2.46	0.48
1:A:32:LEU:O	1:A:36:LEU:HD12	2.14	0.48
1:A:780:THR:HG22	1:B:762:TYR:CZ	2.49	0.48
1:B:710:LEU:HB3	1:B:720:ILE:HD11	1.96	0.48
1:D:1013:PRO:CB	1:D:1015:ARG:HH21	2.26	0.48
1:A:804:GLN:HG3	8:A:1208:HOH:O	2.13	0.48
1:C:172:ARG:NH2	1:C:177:PRO:O	2.44	0.48
1:A:289:LYS:HG3	1:A:441:VAL:HG13	1.95	0.47
1:B:955:ASN:HB3	1:B:978:HIS:HB3	1.95	0.47
1:A:948:ILE:HG12	1:A:1002:ILE:HG12	1.96	0.47
1:A:97:ILE:HA	1:A:100:PHE:CD2	2.50	0.47
1:D:261:LEU:HD12	1:D:266:ILE:O	2.14	0.47
1:B:124:LEU:HD11	1:B:161:GLU:HG2	1.97	0.47
1:A:615:GLU:O	1:B:1015:ARG:HD3	2.15	0.47
1:D:336:ILE:HD11	1:D:429:LEU:HG	1.97	0.47
1:A:776:ARG:HH21	1:B:739:SER:HB3	1.80	0.47
1:D:1013:PRO:HB2	1:D:1015:ARG:HH21	1.80	0.47
1:A:427:VAL:HG13	1:B:410:ARG:HD2	1.97	0.47
1:B:343:THR:HA	3:B:1105:FAD:HM73	1.95	0.47
1:C:374:PRO:HA	1:C:377:VAL:CG1	2.44	0.47
1:A:56:GLU:HB3	1:A:895:MET:HE1	1.97	0.46



		Interatomic		
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:124:LEU:HD13	1:D:160:SER:HB2	1.97	0.46	
1:D:221:GLU:CD	1:D:221:GLU:H	2.17	0.46	
1:B:485:MET:HE1	8:B:1207:HOH:O	2.16	0.46	
1:A:631:ASP:OD2	8:A:1210:HOH:O	2.21	0.46	
1:A:646:ASN:HB3	1:A:649:ASP:HB2	1.97	0.46	
1:B:97:ILE:HA	1:B:100:PHE:CD2	2.51	0.46	
1:A:26:ALA:HB3	1:B:521:LEU:HB2	1.96	0.46	
1:D:921:ILE:O	1:D:925:ILE:HG13	2.15	0.46	
1:A:669:LEU:HD13	1:A:691:VAL:HG22	1.97	0.46	
1:B:413:GLN:HG2	1:B:417:GLY:HA2	1.98	0.46	
1:D:1013:PRO:HB2	1:D:1015:ARG:HE	1.80	0.46	
1:D:353:ARG:NH1	1:D:383:GLU:OE1	2.48	0.46	
1:B:289:LYS:HG3	1:B:441:VAL:HG13	1.98	0.46	
1:A:348:ALA:HB2	1:A:361:LEU:HD21	1.96	0.46	
1:A:806:LEU:O	1:A:925:ILE:HA	2.16	0.46	
1:A:837:LEU:O	1:A:841:LYS:HG3	2.15	0.46	
1:C:366:GLY:H	1:C:369:ASN:ND2	2.14	0.46	
1:A:734:ALA:HA	1:A:735:THR:HA	1.73	0.46	
1:A:741:LEU:HD12	1:B:779:THR:HG21	1.97	0.46	
1:D:122:LEU:HA	1:D:244:GLU:HG2	1.98	0.46	
1:A:364:ARG:H	1:A:364:ARG:CD	2.21	0.46	
1:C:142:LEU:HD12	1:C:150:ILE:HG12	1.98	0.46	
1:D:725:LYS:NZ	8:D:1238:HOH:O	2.47	0.46	
1:D:53:GLU:O	1:D:55:LEU:HG	2.16	0.45	
1:B:237:PRO:HB2	1:B:239:ASP:OD1	2.16	0.45	
1:B:699:ARG:HB2	1:B:728:GLY:HA3	1.98	0.45	
1:C:95:LEU:HD11	1:C:120:ASN:HB2	1.97	0.45	
1:D:267:THR:OG1	1:D:270:THR:HG23	2.14	0.45	
1:D:623:GLN:O	1:D:627:GLU:HG3	2.15	0.45	
1:A:776:ARG:O	1:A:780:THR:HG23	2.17	0.45	
1:C:901:ASN:ND2	8:C:1206:HOH:O	2.11	0.45	
1:C:993:LEU:HD13	1:C:1004:MET:HG2	1.99	0.45	
1:D:669:LEU:HD13	1:D:691:VAL:HG22	1.98	0.45	
1:A:647:LYS:NZ	8:A:1242:HOH:O	2.48	0.45	
1:A:927:LYS:HD3	1:A:927:LYS:HA	1.78	0.45	
1:D:959:CYS:HB2	1:D:992:CYS:HB2	1.98	0.45	
1:C:424:ASP:OD1	1:C:424:ASP:N	2.43	0.45	
1:A:95:LEU:HD22	1:A:116:ILE:HA	1.98	0.45	
1:A:938:LEU:O	8:A:1211:HOH:O	2.21	0.45	
1:C:97:ILE:HA	1:C:100:PHE:CE2	2.52	0.45	
1:A:518:LYS:O	1:A:520:GLU:HG2	2.16	0.45	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:184:GLU:O	1:B:187:SER:OG	2.33	0.45
1:D:789:PRO:HA	8:D:1229:HOH:O	2.16	0.45
1:A:125:THR:O	1:A:129:VAL:HG22	2.16	0.45
1:A:407:GLN:HA	1:A:427:VAL:O	2.17	0.45
1:C:955:ASN:HB3	1:C:978:HIS:HB3	1.98	0.45
1:B:193:LEU:HD11	1:B:266:ILE:HG21	1.99	0.44
1:C:137:VAL:HG13	1:C:149:SER:HB2	1.99	0.44
1:C:365:LYS:HG2	1:C:419:TRP:CZ2	2.52	0.44
1:C:806:LEU:O	1:C:925:ILE:HA	2.17	0.44
1:D:123:GLY:O	1:D:156:GLN:NE2	2.48	0.44
1:C:114:LYS:NZ	1:C:524:PHE:O	2.49	0.44
1:C:875:LYS:HB2	1:C:875:LYS:HE2	1.72	0.44
1:D:831:CYS:O	1:D:835:LYS:HG3	2.17	0.44
1:A:331:ILE:HG23	1:A:433:VAL:HG21	2.00	0.44
1:A:945:VAL:HG13	1:A:1007:ARG:HB2	1.98	0.44
1:D:849:TRP:CG	1:D:854:PRO:HA	2.52	0.44
1:A:269:ASN:O	1:A:273:GLU:HG3	2.17	0.44
1:B:501:TRP:O	1:B:504:HIS:HB3	2.18	0.44
1:B:680:MET:O	1:B:680:MET:HG2	2.17	0.44
1:C:265:GLU:HB3	1:C:266:ILE:H	1.67	0.44
1:C:866:PRO:HG2	1:C:890:ILE:CD1	2.48	0.44
1:A:996:CYS:HB2	1:A:1002:ILE:HD12	2.00	0.44
1:B:758:LYS:HD2	1:B:758:LYS:HA	1.76	0.44
1:C:692:ARG:HB2	1:C:723:ALA:HB1	1.99	0.44
1:C:994:SER:HB3	1:D:592:ARG:HB3	2.00	0.44
1:D:574:LYS:NZ	1:D:612:LEU:O	2.51	0.44
1:B:210:GLY:O	8:B:1208:HOH:O	2.21	0.44
1:C:289:LYS:HG3	1:C:441:VAL:HG13	1.99	0.44
1:D:709:LYS:HD3	5:D:1107:FNR:O2	2.18	0.44
1:D:984:ASP:OD2	1:D:1009:THR:HG21	2.17	0.44
1:A:868:ILE:O	1:A:872:MET:HG3	2.18	0.44
1:B:842:SER:HB2	1:B:916:LYS:O	2.17	0.44
1:C:842:SER:HB2	1:C:916:LYS:O	2.18	0.44
1:B:957:GLY:O	1:B:961:MET:HG3	2.18	0.44
1:C:171:ILE:HG23	1:C:527:PRO:HD3	1.99	0.44
1:C:263:GLU:CG	1:C:449:GLU:HB3	2.48	0.44
1:A:457:ASN:HB3	1:A:463:GLU:HG2	1.99	0.43
1:D:859:HIS:NE2	8:D:1207:HOH:O	2.16	0.43
1:A:966:SER:HA	1:B:553:PRO:HA	2.00	0.43
1:A:373:VAL:HG12	1:B:47:LYS:HD3	1.99	0.43
1:A:261:LEU:O	1:A:447:VAL:HG22	2.19	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:553:PRO:HA	1:B:966:SER:HA	2.00	0.43
1:A:611:GLU:O	4:A:1106:TDR:H6	2.18	0.43
1:A:705:PRO:HA	1:A:730:ASP:OD2	2.19	0.43
1:D:993:LEU:HD13	1:D:1004:MET:HG2	2.01	0.43
1:A:63:LYS:HE3	1:A:128:MET:HG2	2.01	0.43
1:A:550:SER:HB2	1:A:572:LEU:HB3	2.00	0.43
1:A:741:LEU:HD23	1:A:741:LEU:HA	1.88	0.43
1:C:109:TYR:HD2	1:C:162:VAL:HG11	1.84	0.43
1:D:193:LEU:HD13	1:D:217:PHE:HB2	2.01	0.43
1:A:146:GLU:OE1	1:B:70:ARG:NH2	2.52	0.43
1:D:557:SER:H	1:D:620:TYR:HH	1.65	0.43
1:C:331:ILE:HG22	1:C:331:ILE:O	2.18	0.43
1:C:990:THR:O	1:C:990:THR:HG22	2.19	0.43
1:D:114:LYS:NZ	1:D:524:PHE:O	2.51	0.43
1:B:7:LYS:HB2	1:B:7:LYS:HE2	1.46	0.42
1:C:972:GLN:O	1:C:980:PRO:HA	2.19	0.42
1:A:574:LYS:HZ1	5:A:1107:FNR:H5	1.66	0.42
1:A:689:GLU:HG3	1:A:690:LEU:N	2.34	0.42
1:D:124:LEU:HB3	1:D:244:GLU:OE1	2.19	0.42
1:D:783:ARG:HG3	1:D:929:LEU:HD22	2.00	0.42
1:A:329:PRO:O	1:A:354:CYS:HB3	2.19	0.42
1:B:130:CYS:HB2	2:B:1102:SF4:S4	2.53	0.42
1:D:394:ARG:HG3	1:D:409:VAL:HG13	2.00	0.42
1:A:339:GLY:HA2	1:A:364:ARG:NH1	2.34	0.42
1:B:130:CYS:O	1:B:132:THR:HG23	2.19	0.42
1:C:623:GLN:O	1:C:627:GLU:HG3	2.19	0.42
1:D:62:ILE:HD12	1:D:379:LEU:HD12	2.01	0.42
1:A:171:ILE:HG23	1:A:527:PRO:HD3	2.00	0.42
1:A:845:GLU:OE1	1:A:845:GLU:N	2.46	0.42
1:A:900:GLN:NE2	8:A:1248:HOH:O	2.52	0.42
1:C:474:PRO:HB2	1:C:506:TYR:HE2	1.84	0.42
1:A:935:PHE:CE2	1:B:612:LEU:HD11	2.54	0.42
1:B:841:LYS:O	1:B:916:LYS:HE3	2.19	0.42
1:C:738:VAL:HG21	1:C:773:ILE:HD12	2.02	0.42
1:D:537:MET:SD	1:D:811:SER:HB2	2.60	0.42
1:A:451:LEU:O	1:A:454:ILE:HG12	2.20	0.42
1:B:972:GLN:O	1:B:980:PRO:HA	2.19	0.42
1:C:74:ARG:HG3	1:D:599:MET:HE1	2.02	0.42
1:C:263:GLU:HG2	1:C:449:GLU:HB3	2.02	0.42
1:D:172:ARG:HB3	8:D:1226:HOH:O	2.19	0.42
1:A:54:LYS:HD3	1:A:891:ALA:HB1	2.01	0.42



	A + O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:293:ILE:HD12	1:A:394:ARG:O	2.19	0.42
1:A:501:TRP:CE2	1:A:519:PRO:HA	2.54	0.42
1:C:734:ALA:HA	1:C:735:THR:HA	1.72	0.42
1:C:944:VAL:HG22	1:D:587:SER:HB2	2.01	0.42
1:D:846:LEU:HD21	1:D:912:PHE:HE2	1.85	0.42
1:D:868:ILE:HD12	1:D:871:LEU:HD12	2.01	0.42
1:C:219:LYS:HG3	1:C:260:SER:OG	2.18	0.42
1:C:316:SER:HB2	1:C:326:SER:O	2.20	0.42
1:D:231:ILE:HA	1:D:232:PRO:HD3	1.95	0.42
1:B:231:ILE:HA	1:B:232:PRO:HD3	1.95	0.42
1:C:589:ARG:O	1:C:609:ASN:HA	2.20	0.42
1:C:776:ARG:HG3	1:D:762:TYR:CD1	2.54	0.42
1:C:935:PHE:CE2	1:D:612:LEU:HD11	2.55	0.41
1:D:874:LYS:HA	1:D:874:LYS:HD2	1.70	0.41
1:A:608:LEU:HD13	1:A:742:MET:HB2	2.02	0.41
1:A:722:ARG:NH2	8:A:1216:HOH:O	2.28	0.41
1:B:871:LEU:HD22	1:B:886:ARG:HG2	2.02	0.41
1:D:321:MET:HG2	1:D:322:CYS:N	2.33	0.41
1:B:126:CYS:O	1:B:130:CYS:HB2	2.19	0.41
1:B:331:ILE:HD13	1:B:433:VAL:HG21	2.02	0.41
1:D:80:LEU:HD23	1:D:602:PRO:HD3	2.02	0.41
1:A:86:PRO:HA	1:A:89:LYS:HG3	2.02	0.41
1:A:246:GLU:OE1	1:A:909:ARG:HB3	2.21	0.41
1:A:468:THR:HA	1:A:502:TYR:CD2	2.56	0.41
1:B:364:ARG:HD3	1:B:364:ARG:H	1.85	0.41
1:B:501:TRP:CZ2	1:B:519:PRO:HA	2.56	0.41
1:B:822:GLN:NE2	8:B:1203:HOH:O	2.13	0.41
1:A:36:LEU:HD12	1:A:36:LEU:H	1.86	0.41
1:B:183:PRO:HG2	1:B:186:TYR:CE2	2.55	0.41
1:B:993:LEU:HD13	1:B:1004:MET:HG2	2.01	0.41
1:C:41:TRP:CE2	1:D:89:LYS:HD2	2.56	0.41
1:C:73:LEU:HD22	1:D:598:PRO:HG3	2.02	0.41
1:C:960:TYR:CD1	1:C:973:PHE:HB2	2.56	0.41
1:D:589:ARG:HG3	1:D:590:ILE:HG13	2.02	0.41
1:B:734:ALA:HA	1:B:735:THR:HA	1.78	0.41
1:B:62:ILE:CD1	1:B:379:LEU:HD23	2.51	0.41
1:C:407:GLN:HA	1:C:427:VAL:O	2.21	0.41
1:A:533:ILE:O	1:A:545:PRO:HD3	2.21	0.41
1:B:568:TRP:CE2	1:B:827:ILE:HB	2.56	0.41
1:D:988:GLY:HA2	1:D:1004:MET:HE1	2.02	0.41
1:B:225:GLY:HA2	3:B:1105:FAD:H3B	2.03	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:443:ARG:HA	1:B:443:ARG:HD3	1.80	0.41
1:C:6:SER:O	6:SER:O 1:D:561:ARG:NE		0.41
1:D:589:ARG:O	1:D:609:ASN:HA	2.21	0.41
1:A:283:ILE:HG13	1:A:482:ILE:HD13	2.03	0.41
1:A:361:LEU:HD13	1:A:361:LEU:HA	1.96	0.41
1:A:866:PRO:HG2	1:A:890:ILE:HD11	2.02	0.41
1:B:52:CYS:HA	1:B:384:LYS:HG3	2.02	0.41
1:C:47:LYS:NZ	8:C:1249:HOH:O	2.54	0.41
1:C:172:ARG:NH1	1:C:177:PRO:O	2.52	0.41
1:D:293:ILE:HD13	1:D:293:ILE:HA	1.86	0.41
1:A:50:PHE:HD2	1:B:369:ASN:HD22	1.69	0.40
1:A:823:ASP:O	1:A:826:VAL:HG22	2.22	0.40
1:C:834:LEU:HD12	1:C:834:LEU:HA	1.86	0.40
1:D:955:ASN:HB3	1:D:978:HIS:HB3	2.03	0.40
1:B:388:LEU:HB3	1:B:391:LEU:HD12	2.04	0.40
1:B:448:LYS:NZ	1:B:460:ASP:OD2	2.32	0.40
1:B:807:HIS:HB3	1:B:928:ALA:HB2	2.03	0.40
1:B:844:GLU:OE1	1:B:915:LYS:HE2	2.20	0.40
1:B:872:MET:HE2	1:B:872:MET:HB2	1.91	0.40
1:C:109:TYR:CD2	1:C:162:VAL:HG11	2.57	0.40
1:C:457:ASN:HB3	1:C:463:GLU:HG3	2.02	0.40
1:D:20:PRO:HG2	1:D:961:MET:SD	2.61	0.40
1:D:62:ILE:HG12	1:D:234:PHE:HB2	2.03	0.40
1:D:336:ILE:HD13	1:D:336:ILE:HG21	1.90	0.40
1:B:73:LEU:HD23	1:B:73:LEU:HA	1.94	0.40
1:B:593:GLY:HA3	1:B:606:SER:OG	2.21	0.40
1:B:698:VAL:O	1:B:702:VAL:HG22	2.20	0.40
1:D:166:MET:HB3	1:D:168:ILE:HG13	2.04	0.40
1:B:455:LYS:HA	1:B:455:LYS:HD2	1.89	0.40
1:C:305:THR:OG1	1:C:308:ASP:OD2	2.32	0.40
3:C:1105:FAD:H9	3:C:1105:FAD:H1'1	1.86	0.40
1:D:365:LYS:HD3	1:D:419:TRP:CZ2	2.57	0.40
1:D:471:THR:HB	8:D:1254:HOH:O	2.21	0.40
1:D:533:ILE:O	1:D:545:PRO:HD3	2.21	0.40
1:B:90:SER:HB2	1:B:136:CYS:HA	2.04	0.40
1:C:168:ILE:HG22	1:C:526:THR:HB	2.04	0.40
1:D:171:ILE:HD11	1:D:174:PRO:HG3	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)
8:B:1377:HOH:O	8:D:1318:HOH:O[2_545]	2.06	0.14

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	Perce	entiles	5
1	А	1014/1025~(99%)	966 (95%)	43 (4%)	5~(0%)	29	22	
1	В	1014/1025~(99%)	950 (94%)	58 (6%)	6 (1%)	25	17	
1	С	1014/1025~(99%)	954 (94%)	51 (5%)	9 (1%)	17	10	
1	D	1014/1025~(99%)	959~(95%)	48 (5%)	7 (1%)	22	14	
All	All	4056/4100 (99%)	3829 (94%)	200 (5%)	27 (1%)	22	14	

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	677	GLU
1	А	905	PRO
1	В	905	PRO
1	С	905	PRO
1	D	822	GLN
1	А	794	GLY
1	В	728	GLY
1	В	900	GLN
1	D	677	GLU
1	D	905	PRO
1	А	3	PRO
1	А	822	GLN
1	В	677	GLU
1	С	321	MET
1	С	676	GLY
1	С	677	GLU
1	С	902	ALA



Mol	Chain	Res	Type
1	С	903	ALA
1	D	323	ALA
1	В	904	PHE
1	С	3	PRO
1	С	794	GLY
1	D	674	GLY
1	D	906	PRO
1	D	904	PHE
1	В	613	ILE
1	С	613	ILE

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	Perce	ntiles
1	А	840/854~(98%)	813~(97%)	27 (3%)	39	37
1	В	844/854~(99%)	824 (98%)	20~(2%)	49	49
1	С	840/854~(98%)	809~(96%)	31~(4%)	34	31
1	D	844/854~(99%)	820~(97%)	24 (3%)	43	42
All	All	3368/3416 (99%)	3266 (97%)	102 (3%)	41	39

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	11	ASP
1	А	14	SER
1	А	50	PHE
1	А	51	HIS
1	А	74	ARG
1	А	100	PHE
1	А	115	MET
1	А	288	PRO
1	А	363	PHE
1	А	364	ARG
1	А	369	ASN



\mathbf{Mol}	Chain	Res	Type
1	А	392	SER
1	А	404	VAL
1	А	420	ASN
1	А	436	SER
1	А	443	ARG
1	А	448	LYS
1	А	485	MET
1	А	487	ASN
1	А	514	SER
1	А	644	SER
1	А	800	GLU
1	А	844	GLU
1	А	847	GLN
1	А	875	LYS
1	А	895	MET
1	А	916	LYS
1	В	93	THR
1	В	100	PHE
1	В	105	SER
1	В	118	SER
1	В	262	SER
1	В	312	LEU
1	В	363	PHE
1	В	364	ARG
1	В	394	ARG
1	В	399	LYS
1	В	455	LYS
1	В	458	ARG
1	В	574	LYS
1	В	675	MET
1	В	719	SER
1	В	800	GLU
1	В	816	CYS
1	В	874	LYS
1	В	885	GLN
1	В	916	LYS
1	С	7	LYS
1	С	64	HIS
1	С	89	LYS
1	С	100	PHE
1	С	103	SER
1	С	149	SER



Mol	Chain	Res	Type
1	С	167	ASN
1	С	178	SER
1	С	316	SER
1	С	326	SER
1	С	332	ARG
1	С	357	ARG
1	С	363	PHE
1	С	364	ARG
1	С	394	ARG
1	С	410	ARG
1	С	436	SER
1	С	487	ASN
1	С	541	LYS
1	С	608	LEU
1	C	671	SER
1	С	675	MET
1	С	690	LEU
1	С	800	GLU
1	С	874	LYS
1	С	888	LYS
1	С	898	LYS
1	С	927	LYS
1	С	934	THR
1	С	1000	ASP
1	С	1014	LYS
1	D	14	SER
1	D	15	ILE
1	D	39	LYS
1	D	74	ARG
1	D	100	PHE
1	D	130	CYS
1	D	173	ASN
1	D	260	SER
1	D	263	GLU
1	D	330	SER
1	D	338	LEU
1	D	363	PHE
1	D	364	ARG
1	D	436	SER
1	D	487	ASN
1	D	536	GLU
1	D	654	SER



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Mol	Chain	Res	Type
1	D	655	ARG
1	D	671	SER
1	D	696	ARG
1	D	719	SER
1	D	847	GLN
1	D	893	GLU
1	D	916	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	407	GLN
1	В	64	HIS
1	В	220	GLN
1	В	269	ASN
1	В	301	GLN
1	В	693	ASN
1	С	23	GLN
1	С	369	ASN
1	С	648	ASN
1	С	700	GLN
1	D	173	ASN
1	D	407	GLN
1	D	693	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 monosaccharides 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	Dog	Link	В	ond leng	gths	Bond angles		
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
6	FMN	С	1106	-	33,33,33	1.01	2 (6%)	48,50,50	1.22	7 (14%)
2	SF4	В	1101	1	0,12,12	-	-	-		
2	SF4	С	1101	1	0,12,12	-	-	-		
3	FAD	D	1105	-	53,58,58	0.46	0	68,89,89	0.48	1 (1%)
5	FNR	А	1107	-	32,33,33	4.09	17 (53%)	40,50,50	1.56	8 (20%)
2	SF4	С	1103	1	0,12,12	-	-	-		
2	SF4	А	1101	1	$0,\!12,\!12$	-	-	-		
2	SF4	С	1104	1	$0,\!12,\!12$	-	-	-		
2	SF4	А	1103	1	0,12,12	-	-	-		
2	SF4	В	1102	1	$0,\!12,\!12$	-	-	-		
3	FAD	С	1105	-	53,58,58	0.45	0	68,89,89	0.52	1 (1%)
7	XH5	C	1107	-	$8,\!9,\!9$	6.37	6 (75%)	8,12,12	2.49	4 (50%)
2	SF4	В	1103	1	0,12,12	-	-	-		
4	TDR	D	1106	-	9,9,9	0.44	0	12,12,12	0.65	0
2	SF4	С	1102	1	0,12,12	-	-	-		
2	SF4	D	1103	1	0,12,12	-	-	-		
6	FMN	В	1106	-	33,33,33	1.05	2 (6%)	48,50,50	1.22	7 (14%)
2	SF4	А	1102	1	0,12,12	-	-	-		
2	SF4	D	1101	1	0,12,12	-	-	-		
5	FNR	D	1107	-	32,33,33	4.03	17 (53%)	40,50,50	1.48	7 (17%)
7	XH5	В	1107	-	$8,\!9,\!9$	<mark>6.38</mark>	6 (75%)	8,12,12	2.46	4 (50%)
2	SF4	D	1104	1	$0,\!12,\!12$	-	-	-		
4	TDR	A	1106	-	$9,\!9,\!9$	0.42	0	12,12,12	0.66	0
3	FAD	В	1105	-	$53,\!58,\!58$	0.46	0	68,89,89	0.46	1 (1%)
2	SF4	A	1104	1	0,12,12	-	-	-		
2	SF4	В	1104	1	$0,\!12,\!12$	-		-		
2	SF4	D	1102	1	0,12,12	-	-	-		
3	FAD	A	1105	-	53,58,58	0.47	0	68,89,89	0.48	1 (1%)



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
6	FMN	С	1106	-	-	6/18/18/18	0/3/3/3
2	SF4	В	1101	1	-	-	0/6/5/5
2	SF4	С	1101	1	-	-	0/6/5/5
3	FAD	D	1105	-	-	5/30/50/50	0/6/6/6
5	FNR	А	1107	-	-	7/18/18/18	0/3/3/3
2	SF4	С	1103	1	-	-	0/6/5/5
2	SF4	А	1101	1	-	-	0/6/5/5
2	SF4	А	1103	1	-	-	0/6/5/5
2	SF4	С	1104	1	-	-	0/6/5/5
2	SF4	В	1102	1	-	-	0/6/5/5
3	FAD	С	1105	-	-	1/30/50/50	0/6/6/6
7	XH5	С	1107	-	-	-	0/1/1/1
2	SF4	В	1103	1	-	-	0/6/5/5
4	TDR	D	1106	-	-	-	0/1/1/1
2	SF4	С	1102	1	-	-	0/6/5/5
2	SF4	D	1103	1	-	-	0/6/5/5
6	FMN	В	1106	-	-	1/18/18/18	0/3/3/3
2	SF4	А	1102	1	-	-	0/6/5/5
2	SF4	D	1101	1	-	-	0/6/5/5
5	FNR	D	1107	_	-	1/18/18/18	0/3/3/3
7	XH5	В	1107	-	-	-	0/1/1/1
2	SF4	D	1104	1	-	-	0/6/5/5
4	TDR	А	1106	-	-	-	0/1/1/1
3	FAD	В	1105	-	-	6/30/50/50	0/6/6/6
2	SF4	А	1104	1	-	-	0/6/5/5
2	SF4	В	1104	1	-	-	0/6/5/5
2	SF4	D	1102	1	-	-	0/6/5/5
3	FAD	А	1105	-	-	7/30/50/50	0/6/6/6

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	С	1107	XH5	C02-N01	14.95	1.50	1.34
7	В	1107	XH5	C02-N01	14.84	1.50	1.34
5	А	1107	FNR	C9-C9A	8.34	1.53	1.39
5	D	1107	FNR	C9-C9A	8.29	1.53	1.39
5	D	1107	FNR	O4-C4	8.25	1.39	1.23
5	А	1107	FNR	O4-C4	8.20	1.39	1.23



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	А	1107	FNR	C6-C5A	8.07	1.52	1.39
7	В	1107	XH5	C02-N04	7.91	1.51	1.37
5	D	1107	FNR	C6-C5A	7.83	1.51	1.39
7	С	1107	XH5	C02-N04	7.74	1.50	1.37
5	А	1107	FNR	O2-C2	7.50	1.39	1.23
5	D	1107	FNR	O2-C2	7.46	1.39	1.23
5	D	1107	FNR	C5A-C9A	-7.16	1.32	1.40
5	А	1107	FNR	C5A-C9A	-7.06	1.32	1.40
5	А	1107	FNR	CAA-N1	6.31	1.48	1.37
5	D	1107	FNR	CAA-N1	6.25	1.48	1.37
5	А	1107	FNR	C2-N1	5.17	1.46	1.37
5	А	1107	FNR	C5A-N5	5.15	1.48	1.39
5	D	1107	FNR	C5A-N5	4.99	1.48	1.39
5	D	1107	FNR	C2-N1	4.98	1.46	1.37
7	В	1107	XH5	C05-N04	4.86	1.45	1.37
7	С	1107	XH5	C05-N04	4.64	1.45	1.37
5	А	1107	FNR	C4A-N5	4.56	1.45	1.35
5	А	1107	FNR	C4A-C4	4.51	1.53	1.42
5	D	1107	FNR	C4A-N5	4.46	1.45	1.35
5	D	1107	FNR	C4A-C4	4.41	1.53	1.42
5	А	1107	FNR	C9A-N10	4.24	1.48	1.41
5	А	1107	FNR	C2-N3	4.09	1.44	1.37
5	D	1107	FNR	C2-N3	3.96	1.44	1.37
5	D	1107	FNR	C9A-N10	3.86	1.47	1.41
6	В	1106	FMN	C4A-N5	3.80	1.38	1.30
6	С	1106	FMN	C4A-N5	3.62	1.37	1.30
5	А	1107	FNR	CAA-N10	3.61	1.44	1.38
5	D	1107	FNR	CAA-N10	3.49	1.44	1.38
7	С	1107	XH5	C08-C07	2.83	1.62	1.52
7	В	1107	XH5	C08-C07	2.78	1.62	1.52
5	A	1107	FNR	C4-N3	2.70	1.43	1.38
5	D	1107	FNR	C4-N3	2.61	1.43	1.38
6	В	1106	FMN	C10-N1	2.52	1.38	1.33
6	С	1106	FMN	C10-N1	2.43	1.38	1.33
7	С	1107	XH5	O06-C05	-2.40	1.18	1.23
7	B	1107	XH5	O06-C05	-2.20	1.19	1.23
5	A	1107	FNR	P-O3P	-2.19	1.46	1.54
7	B	1107	XH5	003-C02	-2.16	1.18	1.23
5	A	1107	FNR	P-01P	-2.16	1.46	1.54
5	D	1107	FNR	P-O3P	-2.12	1.46	1.54
5	A	1107	FNR	C8M-C8	2.12	1.55	1.51
7	\mathbf{C}	1107	XH5	O03-C02	-2.10	1.19	1.23



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	D	1107	FNR	C8M-C8	2.09	1.55	1.51
5	D	1107	FNR	P-O1P	-2.02	1.47	1.54

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
7	С	1107	XH5	C05-N04-C02	-4.96	119.61	126.25
5	А	1107	FNR	C4-N3-C2	-4.92	119.25	126.34
7	В	1107	XH5	C05-N04-C02	-4.64	120.04	126.25
5	D	1107	FNR	C4-N3-C2	-4.63	119.67	126.34
5	А	1107	FNR	O4-C4-C4A	-3.72	118.72	127.24
5	D	1107	FNR	O4-C4-C4A	-3.61	118.97	127.24
6	С	1106	FMN	C4-N3-C2	-3.22	119.69	125.64
5	D	1107	FNR	O5'-P-O2P	3.15	115.32	106.47
6	В	1106	FMN	C4-N3-C2	-3.10	119.92	125.64
5	D	1107	FNR	O1P-P-O5'	3.07	114.90	106.73
5	А	1107	FNR	C5'-C4'-C3'	-2.94	106.53	112.20
7	В	1107	XH5	N04-C02-N01	2.92	120.03	116.61
7	С	1107	XH5	N04-C02-N01	2.89	119.99	116.61
7	В	1107	XH5	C09-C07-C05	2.81	119.59	111.53
6	В	1106	FMN	O4-C4-C4A	-2.80	119.19	126.60
7	С	1107	XH5	C09-C07-C05	2.78	119.50	111.53
5	А	1107	FNR	O1P-P-O5'	2.77	114.09	106.73
5	А	1107	FNR	O5'-P-O2P	2.73	114.12	106.47
6	В	1106	FMN	C4A-C4-N3	2.69	120.02	113.19
6	С	1106	FMN	O4-C4-C4A	-2.68	119.49	126.60
5	А	1107	FNR	O3P-P-O5'	2.67	113.84	106.73
6	С	1106	FMN	C4A-C4-N3	2.65	119.91	113.19
7	В	1107	XH5	C08-C07-C09	-2.60	106.65	112.06
5	А	1107	FNR	N3-C2-N1	2.55	119.91	115.80
7	С	1107	XH5	C08-C07-C09	-2.40	107.05	112.06
5	D	1107	FNR	N3-C2-N1	2.40	119.65	115.80
5	А	1107	FNR	C4A-C4-N3	2.39	119.44	112.31
6	С	1106	FMN	C4A-C10-N10	2.35	119.92	116.48
3	В	1105	FAD	C5A-C6A-N6A	2.35	123.92	120.35
5	D	1107	FNR	C4A-C4-N3	2.33	119.25	112.31
3	D	1105	FAD	C5A-C6A-N6A	2.32	123.88	120.35
3	С	1105	FAD	C5A-C6A-N6A	2.31	123.86	120.35
3	A	1105	FAD	C5A-C6A-N6A	2.28	123.82	120.35
6	В	1106	FMN	C4A-C10-N10	2.25	119.76	116.48
6	С	1106	FMN	C10-C4A-N5	-2.23	120.13	124.86
5	D	1107	FNR	O3P-P-O5'	2.20	112.60	106.73



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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	В	1106	FMN	C10-C4A-N5	-2.18	120.23	124.86
6	В	1106	FMN	C4A-C10-N1	-2.18	119.68	124.73
6	С	1106	FMN	C4A-C10-N1	-2.14	119.76	124.73
6	В	1106	FMN	C9A-C5A-N5	-2.07	120.18	122.43
6	С	1106	FMN	C9A-C5A-N5	-2.05	120.20	122.43

There are no chirality outliers.

All	(34)	$\operatorname{torsion}$	outliers	are	listed	below:

Mol	Chain	Res	Type	Atoms
3	В	1105	FAD	O4'-C4'-C5'-O5'
5	А	1107	FNR	C2'-C3'-C4'-C5'
5	А	1107	FNR	O3'-C3'-C4'-C5'
5	А	1107	FNR	O3'-C3'-C4'-O4'
3	D	1105	FAD	O4B-C4B-C5B-O5B
5	А	1107	FNR	C2'-C3'-C4'-O4'
3	А	1105	FAD	O4B-C4B-C5B-O5B
3	D	1105	FAD	C3B-C4B-C5B-O5B
3	А	1105	FAD	C2'-C3'-C4'-O4'
5	А	1107	FNR	C5'-O5'-P-O2P
3	А	1105	FAD	O3'-C3'-C4'-O4'
5	А	1107	FNR	C4'-C5'-O5'-P
3	В	1105	FAD	PA-O3P-P-O5'
3	А	1105	FAD	C5'-O5'-P-O3P
3	D	1105	FAD	C5'-O5'-P-O3P
5	D	1107	FNR	C4'-C5'-O5'-P
3	А	1105	FAD	C3B-C4B-C5B-O5B
3	А	1105	FAD	O3'-C3'-C4'-C5'
6	С	1106	FMN	C5'-O5'-P-O1P
6	В	1106	FMN	C4'-C5'-O5'-P
3	А	1105	FAD	C2'-C3'-C4'-C5'
3	С	1105	FAD	O4B-C4B-C5B-O5B
3	В	1105	FAD	P-O3P-PA-O1A
6	С	1106	FMN	C2'-C3'-C4'-O4'
5	А	1107	FNR	C5'-O5'-P-O1P
6	С	1106	FMN	C5'-O5'-P-O2P
6	С	1106	FMN	C2'-C3'-C4'-C5'
3	В	1105	FAD	O4B-C4B-C5B-O5B
3	В	1105	FAD	P-O3P-PA-O2A
3	В	1105	FAD	C3'-C4'-C5'-O5'
3	D	1105	FAD	C5B-O5B-PA-O1A
3	D	1105	FAD	C5'-O5'-P-O1P



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Mol	Chain	\mathbf{Res}	Type	Atoms
6	С	1106	FMN	O3'-C3'-C4'-C5'
6	С	1106	FMN	C4'-C5'-O5'-P

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1105	FAD	2	0
5	А	1107	FNR	3	0
2	В	1102	SF4	2	0
3	С	1105	FAD	3	0
5	D	1107	FNR	2	0
4	А	1106	TDR	1	0
3	В	1105	FAD	3	0
2	D	1102	SF4	1	0
3	А	1105	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.




























































































5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	А	1007/1025~(98%)	-0.00	34 (3%) 45 52	16, 27, 62, 99	0
1	В	1006/1025~(98%)	0.10	40 (3%) 38 46	14, 29, 62, 130	0
1	С	1007/1025~(98%)	0.04	38 (3%) 40 48	16, 29, 59, 104	0
1	D	1006/1025~(98%)	0.06	41 (4%) 37 45	17, 28, 64, 109	0
All	All	4026/4100 (98%)	0.05	153 (3%) 40 48	14, 28, 63, 130	0

All (153) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	В	870	GLU	15.7
1	D	324	CYS	15.3
1	В	867	ARG	13.3
1	В	869	ALA	13.2
1	В	52	CYS	12.0
1	А	907	LEU	11.5
1	А	2	ALA	11.2
1	А	868	ILE	10.9
1	С	52	CYS	10.9
1	В	868	ILE	9.4
1	D	866	PRO	9.2
1	В	907	LEU	8.9
1	В	902	ALA	8.5
1	С	2	ALA	8.5
1	С	907	LEU	8.5
1	D	51	HIS	8.3
1	D	867	ARG	8.3
1	D	323	ALA	8.2
1	D	52	CYS	8.1
1	С	868	ILE	7.9
1	С	870	GLU	7.8



8	F	6	1
8	F	0	T

Mol	Chain	Res	Type	RSRZ
1	А	869	ALA	7.7
1	В	901	ASN	7.3
1	С	869	ALA	7.1
1	С	50	PHE	7.1
1	В	871	LEU	7.0
1	В	897	LEU	6.8
1	С	871	LEU	6.8
1	А	867	ARG	6.7
1	D	907	LEU	6.7
1	D	673	HIS	6.6
1	D	870	GLU	6.5
1	В	866	PRO	6.3
1	В	865	VAL	6.2
1	D	908	GLU	6.0
1	В	51	HIS	6.0
1	В	900	GLN	5.9
1	А	897	LEU	5.9
1	С	867	ARG	5.8
1	А	902	ALA	5.8
1	А	900	GLN	5.8
1	А	899	GLU	5.6
1	С	674	GLY	5.4
1	С	51	HIS	5.4
1	С	873	GLY	5.4
1	С	900	GLN	5.3
1	В	50	PHE	5.3
1	В	324	CYS	5.3
1	А	414	ASP	5.2
1	В	908	GLU	5.1
1	D	868	ILE	5.1
1	А	50	PHE	5.1
1	D	865	VAL	5.0
1	В	48	ASN	5.0
1	D	680	MET	5.0
1	С	899	GLU	4.9
1	D	417	GLY	4.9
1	D	869	ALA	4.8
1	В	856	THR	4.7
1	С	901	ASN	4.6
1	С	902	ALA	4.5
1	В	673	HIS	4.5
1	D	367	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	319	ALA	4.4
1	А	866	PRO	4.4
1	С	673	HIS	4.4
1	D	322	CYS	4.3
1	D	320	GLY	4.2
1	В	899	GLU	4.1
1	В	681	GLY	4.1
1	В	859	HIS	4.1
1	А	901	ASN	4.1
1	С	908	GLU	4.0
1	С	675	MET	4.0
1	D	900	GLN	4.0
1	А	864	PRO	4.0
1	А	52	CYS	3.9
1	D	873	GLY	3.8
1	А	419	TRP	3.7
1	А	871	LEU	3.7
1	С	53	GLU	3.7
1	В	672	PRO	3.6
1	В	680	MET	3.6
1	С	415	GLU	3.6
1	D	325	HIS	3.5
1	С	681	GLY	3.5
1	D	332	ARG	3.4
1	А	675	MET	3.4
1	А	324	CYS	3.4
1	А	415	GLU	3.4
1	А	325	HIS	3.3
1	С	898	LYS	3.3
1	D	871	LEU	3.3
1	В	130	CYS	3.3
1	D	897	LEU	3.3
1	D	856	THR	3.2
1	D	681	GLY	3.2
1	D	418	LYS	3.1
1	D	899	GLU	3.1
1	С	866	PRO	3.1
1	С	865	VAL	3.1
1	С	48	ASN	3.1
1	А	896	ARG	3.0
1	В	459	TRP	2.9
1	А	908	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	А	873	GLY	2.9
1	С	909	ARG	2.9
1	С	1010	PRO	2.8
1	С	1011	TYR	2.8
1	D	416	THR	2.8
1	D	50	PHE	2.8
1	D	902	ALA	2.7
1	В	46	ASP	2.7
1	В	323	ALA	2.7
1	С	895	MET	2.7
1	В	873	GLY	2.6
1	С	323	ALA	2.6
1	В	53	GLU	2.6
1	D	864	PRO	2.6
1	D	874	LYS	2.6
1	С	459	TRP	2.5
1	D	331	ILE	2.5
1	В	857	GLU	2.5
1	А	416	THR	2.4
1	А	51	HIS	2.4
1	D	1012	GLU	2.4
1	С	319	ALA	2.4
1	С	856	THR	2.4
1	В	582	ILE	2.3
1	D	672	PRO	2.3
1	В	1017	LEU	2.3
1	В	420	ASN	2.3
1	В	1010	PRO	2.3
1	А	870	GLU	2.2
1	D	901	ASN	2.2
1	В	330	SER	2.2
1	\mathbf{C}	855	GLY	2.2
1	С	414	ASP	2.2
1	A	323	ALA	2.2
1	В	1018	PRO	2.2
1	D	53	GLU	2.2
1	A	374	PRO	2.2
1	В	896	ARG	2.2
1	A	859	HIS	2.2
1	А	856	THR	2.1
1	А	368	VAL	2.1
1	D	857	GLU	2.1

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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 monosaccharides 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. 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	$B-factors(Å^2)$	Q<0.9
5	FNR	D	1107	31/31	0.96	0.12	17,24,28,33	0
7	XH5	В	1107	9/9	0.96	0.13	22,27,29,33	0
7	XH5	С	1107	9/9	0.96	0.15	19,24,29,37	0
3	FAD	С	1105	53/53	0.97	0.11	18,27,34,38	0
3	FAD	D	1105	53/53	0.97	0.10	17,23,29,36	0
4	TDR	А	1106	9/9	0.97	0.08	20,23,26,27	0
4	TDR	D	1106	9/9	0.97	0.09	17,22,26,28	0
5	FNR	А	1107	31/31	0.97	0.12	16,25,30,32	0
2	SF4	В	1102	8/8	0.97	0.12	21,23,26,29	0
6	FMN	В	1106	31/31	0.97	0.11	12,23,28,31	0
6	FMN	С	1106	31/31	0.97	0.11	17,27,30,31	0
3	FAD	А	1105	53/53	0.97	0.11	18,24,30,31	0
3	FAD	В	1105	53/53	0.97	0.10	17,26,31,35	0
2	SF4	А	1101	8/8	0.98	0.10	18,21,22,23	0
2	SF4	В	1103	8/8	0.98	0.11	19,23,23,24	0
2	SF4	С	1101	8/8	0.98	0.09	20,21,25,27	0
2	SF4	C	1104	8/8	0.98	0.10	19,24,26,31	0



Chain RSRZ Mol \mathbf{Res} Type MET 1 D 872 2.11 372 А ALA 2.1В 1 874 LYS 2.11 С 340 ALA 2.0VAL 1 А 865 2.01 С 372ALA 2.0

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Mol		Chain	Res	Atoms	BSCC	RSR	B -factors $(Å^2)$	$\Omega < 0.9$
WIOI	Type	Onam	1005	11001115	10000	Itort	\mathbf{D} -lactors(\mathbf{H})	Q < 0.0
2	SF4	D	1101	8/8	0.98	0.11	$18,\!23,\!25,\!25$	0
2	SF4	D	1102	8/8	0.98	0.10	13,18,20,21	0
2	SF4	А	1103	8/8	0.98	0.10	21,24,28,28	0
2	SF4	А	1104	8/8	0.98	0.10	21,23,27,28	0
2	SF4	В	1101	8/8	0.98	0.10	17,19,21,22	0
2	SF4	С	1103	8/8	0.99	0.10	19,25,25,34	0
2	SF4	В	1104	8/8	0.99	0.10	19,21,22,23	0
2	SF4	А	1102	8/8	0.99	0.10	19,21,24,28	0
2	SF4	С	1102	8/8	0.99	0.09	19,20,23,27	0
2	SF4	D	1103	8/8	0.99	0.11	19,22,26,27	0
2	SF4	D	1104	8/8	0.99	0.09	21,23,27,29	0

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The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.






































































































6.5 Other polymers (i)

There are no such residues in this entry.

