

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 15, 2023 – 03:55 PM EDT

PDB ID	:	1TLL
Title	:	CRYSTAL STRUCTURE OF RAT NEURONAL NITRIC-OXIDE SYN-
		THASE REDUCTASE MODULE AT 2.3 A RESOLUTION.
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Deposited on	:	2004-06-09
Resolution	:	2.30  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	:	2.35
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)	:	2.35

# 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 2.30 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	5042(2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575(2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	688	55%	31%	5%	8%				
1	В	688	47%	39%	•	10%				



## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10408 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 Nitric-oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	630	Total 5010	C 3170	N 882	O 932	S 26	0	0	0
1	В	616	Total 4903	C 3106	N 862	O 909	S 26	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1008	SER	PHE	SEE REMARK 999	UNP P29476
В	3008	SER	PHE	SEE REMARK 999	UNP P29476

• Molecule 2 is SULFITE ION (three-letter code: SO3) (formula: O<sub>3</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	А	1	Total 4	O 3	S 1	0	0



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	В	1	Total 4	O 3	S 1	0	0

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



Mol	Chain	Residues		Ato	oms		ZeroOcc	AltConf	
2	Δ	1	Total	С	Ν	0	Р	0	0
D A	L	31	17	4	9	1	0	0	
9	D	1	Total	С	Ν	Ο	Р	0	0
3	D		31	17	4	9	1	0	

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





Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	
4	Δ	1	Total	С	Ν	0	Р	0	0
	T	53	27	9	15	2	0	0	
4	Р	1	Total	С	Ν	0	Р	0	0
4	D	L	53	27	9	15	2	0	0

• Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	
5	Δ	1	Total	С	Ν	Ο	Р	0	0
5	A	1	48	21	7	17	3	0	0



Continued from previous page...

Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	
5	В	1	Total	C 21	N 7	0 17	Р з	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	127	Total O 127 127	0	0
6	В	96	Total O 96 96	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: Nitric-oxide synthase, brain



ALA	LYS	MET	GLY	GLN	ALA MET	ALA	LYS	V2753	K2754	A2755	T2756	12757	L2/58	A2760	T2761	E2762		K2765	99/7.9	Y2769		L2773	C2774	E2775	12//6 F9777	K2778	H2779	A2780	F 2/ 81	A2783	K2784	M2786	S2787	M2788	E2789	Y2791	D2792	I 2793	N 2/ 94 H27 95	L2796		E2799	L2801	V2802	L2803 V2804	V2805	T2806
-	P2815	E2010 N2817	G2818	E2819	K2820 F2821	G2822	C2823	A 20 24	M2826	E2827	M2828	R2829	STH	ASN	SER	VAL	GLN	GLU	GLU ABG	LYS	S2840	Y2841	K2842	V2843	K2844	r 2030 N2846	SER	VAL	SER	TYR	SER	SEB	ARG	LYS	SER	GLY	ASP	GLY	ASP	LEU	ARG	ASP	PHE	GLU	SER THR	GLY	PRO
LEU	ALA		R2878	F2879	52880 V2881	F2882	G2883 1 7004	P 2004	Y2889	P2890	H2891	-	A.2894	r 2030	A2898	V2899		L2902	L2903	E2905	L2906	-	E2909	R2910	12911	K2913	M2914	R2915	F.2919	L2920	C2921	6.29.22	R2928	T2929	W2930 A 2031		V2934	F2935	N 29 30	<mark>C2939</mark>	D2940	V2941	C2943	V2944	G2945 D2946	D2947	V2948
N2949	I2950	E2301 K2952	PRO	ASN	SER	LEU	ILE SODED	N2960	D2961	R2962	S2963	W2964	K2965	N2967	K2968	F2969	R2970	L2971	27972	V2974	A2975	E2976		D2979	L2980 T0081	10271	A2994	A2995	1.2997	L2998	S2999	R3000	N3002	L3003	u3004	<b>S3008</b>	S3009	R3010	F3014	V3015		T3019 N3020	G3021	N3022	1.30.25	<b>q</b> 3026	-
L3033	G3034	H3040	-	V3044	E3049	<b>R3050</b>	L3051		A3054	P3055	P3056	A3057	N3058		K3062	V3063	E3064	M3065	L3066	E3068	R3069	N3070	T3071	A3072	L30/3	13076	S3077	N3078	W3079 K3080	D3081		13089 13090	F3091	<mark>03092</mark>	D3103	P3104		L3107	u3108 L3109	<mark>Q3110</mark>	<b>Q3111</b>	F3112 A3113	S3114	L3115	A3116	E3119	K3120
E3121	K3122	43123 R3124	L3125	L3126	V3127	K3130	G3131 12122	03133 03133	E3134	Y3135	E3136	E3137	1194 40	OTTCM	P3144	<b>T3145</b>	M3146	V3147	E3148 V3140	CH TO A	03157	M3158	P3159	A3160	13161 13162		T3165	Q3166		Q3171		Y3175	S3176		S3180	V3188	H3189		13194 13194	V3195	S3196	Y3197 H3108		D3201	<b>G3202</b>	W3214	-
I3218	03219	D3221	-	C3226	R3238	N3239	P3240	45241 V3242	P3243	C3244	I3245	L3246	V324 /	G3250	T3251	G3252	I3253		K3251	W3260	<b>Q3261</b>	<mark>03262</mark>		D3266	M2070	21201	V3280	F3281	G3282 C3283	R3284	Q3285	53286 K3287	I3288	D3289	43000		V3304	F3305	R3307 E3307	L3308	Y3309	V3310	S3313	R3314	E3315	D3317	R3318
P3319	K3320	Y3322	V3323	03324 20205	U3325 V3326	L3327	03328 82320	E2029	L3331	A3332		V3335	13336	A3338		E3341	<b>Q3342</b>	G3343	63344 H2345	13346	Y3347	V3348	C3349	G3350	U3351 V2357	T3353		L3359	A3361	13362	<mark>03363</mark>	K3365	M3366	T3367	13368 13360	<b>G</b> 3370	K3371	L3372	E3374	E3375	D3376	A3377	V3379	F3380	13381 33382	R3383	L3384
R3385	D3386	R3389	Y3390	H3391	<mark>G3396</mark>	V3397	T3398 123200	L3339 R3400	T3401	Y3402	E3403	V3404	13405	R3407	L3408	R3409	S3410	E3411	53412 T3413	ALA	PHE	ILE	GLU	GLU	SER 1 VS	LYS	ASP	ALA	GL.IJ	VAL	PHE	SER															



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	65.76Å 69.17Å 82.63Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$76.80^{\circ}$ $72.07^{\circ}$ $67.14^{\circ}$	Depositor
$\mathbf{B}_{\mathrm{ascolution}}(\hat{\boldsymbol{\lambda}})$	35.21 - 2.30	Depositor
Resolution (A)	35.21 - 2.17	EDS
% Data completeness	97.8 (35.21-2.30)	Depositor
(in resolution range)	95.5(35.21-2.17)	EDS
$R_{merge}$	(Not available)	Depositor
R <sub>sym</sub>	0.07	Depositor
$< I/\sigma(I) > 1$	$1.61 (at 2.18 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
P. P.	0.244 , $0.272$	Depositor
$\Pi, \Pi_{free}$	0.237 , $0.262$	DCC
$R_{free}$ test set	1909 reflections $(2.98\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	37.4	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , $55.4$	EDS
L-test for $twinning^2$	$ < L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10408	wwPDB-VP
Average B, all atoms $(Å^2)$	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: FMN, NAP, FAD, SO3  $\,$ 

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	Bo	nd lengths	Bond angles				
INIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5			
1	А	0.43	2/5122~(0.0%)	0.71	2/6932~(0.0%)			
1	В	0.40	0/5014	0.76	6/6788~(0.1%)			
All	All	0.41	2/10136~(0.0%)	0.73	8/13720 (0.1%)			

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
1	А	1133	GLN	CA-CB	-5.70	1.41	1.53
1	А	1133	GLN	CG-CD	-5.18	1.39	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	3364	ARG	NE-CZ-NH1	19.58	130.09	120.30
1	В	3364	ARG	NE-CZ-NH2	-16.65	111.97	120.30
1	В	2944	VAL	N-CA-C	-6.22	94.21	111.00
1	В	2966	ARG	N-CA-C	5.69	126.37	111.00
1	В	3364	ARG	CD-NE-CZ	5.38	131.14	123.60
1	А	1133	GLN	CB-CG-CD	-5.15	98.22	111.60
1	В	2943	CYS	N-CA-C	5.06	124.67	111.00
1	А	944	VAL	N-CA-C	-5.01	97.47	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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	5010	0	4925	260	1
1	В	4903	0	4814	287	1
2	А	4	0	0	0	0
2	В	4	0	0	0	0
3	А	31	0	18	0	0
3	В	31	0	18	0	0
4	А	53	0	28	0	0
4	В	53	0	28	0	0
5	А	48	0	24	9	0
5	В	48	0	24	13	0
6	А	127	0	0	2	0
6	В	96	0	0	6	0
All	All	10408	0	9879	545	1

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.

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 27.

All (545) 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)
5:A:1453:NAP:O2A	5:A:1453:NAP:O3D	1.55	1.21
1:B:3360:LYS:O	1:B:3364:ARG:CD	1.98	1.11
1:B:3196:SER:N	6:B:6093:HOH:O	1.59	1.10
1:A:991:ARG:HG3	1:A:991:ARG:HH11	1.12	1.08
1:B:3053:ASP:HB2	1:B:3160:ALA:H	1.11	1.06
1:B:3360:LYS:O	1:B:3364:ARG:HD3	1.54	1.04
1:A:1161:THR:O	1:A:1165:THR:HG22	1.56	1.04
1:B:3324:GLN:H	1:B:3324:GLN:HE21	1.04	1.00
1:B:3398:THR:O	5:B:2453:NAP:O2D	1.80	1.00
1:A:1328:GLN:HE21	1:A:1361:ALA:HA	1.22	0.99
1:A:1078:ASN:N	1:A:1078:ASN:HD22	1.62	0.97
1:B:3313:SER:HB2	1:B:3320:LYS:HE2	1.45	0.96
1:A:1071:THR:HG22	1:A:1072:ALA:H	1.30	0.96
1:B:3360:LYS:HB3	1:B:3364:ARG:NH1	1.81	0.95
1:B:3019:THR:HG23	1:B:3025:LEU:HD12	1.50	0.94
1:B:2843:VAL:HG23	1:B:3386:ASP:OD2	1.68	0.94
1:A:1324:GLN:H	1:A:1324:GLN:HE21	1.08	0.93
1:B:2799:GLU:O	1:B:2877:VAL:HG22	1.70	0.92
1:B:3324:GLN:H	1:B:3324:GLN:NE2	1.68	0.92



	AL O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1324:GLN:HE22	5:A:1453:NAP:H2A	1.34	0.91
1:B:3193:ALA:HB1	5:B:2453:NAP:H51N	1.55	0.89
1:A:991:ARG:HH11	1:A:991:ARG:CG	1.87	0.88
1:A:1071:THR:HG22	1:A:1072:ALA:N	1.89	0.87
1:B:2930:TRP:O	1:B:2934:VAL:HG23	1.74	0.87
1:A:797:GLU:HG3	1:A:798:HIS:CD2	2.10	0.86
1:B:2881:VAL:HB	1:B:2914:MET:HG3	1.54	0.86
1:A:840:SER:OG	1:A:843:VAL:HG23	1.75	0.86
1:B:3283:CYS:HB2	1:B:3289:ASP:HB3	1.58	0.85
1:A:964:TRP:CZ2	1:A:966:ARG:HG3	2.11	0.85
1:A:1309:TYR:CZ	1:A:1331:LEU:HD21	2.11	0.84
1:A:912:LEU:HD22	1:A:915:ARG:HH12	1.41	0.84
1:A:1379:VAL:O	1:A:1383:ARG:HG2	1.77	0.83
1:B:2912:LEU:HD21	1:B:2915:ARG:NH1	1.93	0.83
1:A:775:GLU:HG2	1:A:961:ASP:CB	2.09	0.83
1:A:823:CYS:O	1:A:827:GLU:HG2	1.77	0.83
1:B:2922:GLY:N	1:B:3136:GLU:OE2	2.11	0.82
1:A:1069:ARG:HG2	1:A:1070:ASN:H	1.44	0.82
1:B:3353:THR:HG22	5:B:2453:NAP:H62A	1.44	0.81
1:A:972:THR:HG21	1:A:1064:GLU:OE1	1.80	0.81
1:A:1324:GLN:H	1:A:1324:GLN:NE2	1.79	0.81
1:B:3324:GLN:HE21	1:B:3324:GLN:N	1.76	0.81
1:A:1062:LYS:HE3	1:A:1087:PRO:HG3	1.62	0.80
1:B:3360:LYS:O	1:B:3364:ARG:HD2	1.78	0.80
1:A:1328:GLN:NE2	1:A:1361:ALA:HA	1.96	0.80
1:A:1324:GLN:HE21	1:A:1324:GLN:N	1.80	0.79
1:B:2842:LYS:HD3	1:B:2846:ASN:HD22	1.47	0.79
1:A:1048:ILE:HG21	1:A:1057:ALA:HB2	1.64	0.79
1:A:1328:GLN:NE2	1:A:1364:ARG:HD2	1.98	0.79
1:B:2792:ASP:HB3	1:B:2794:VAL:HG12	1.66	0.78
1:A:1372:LEU:HB3	1:A:1376:ASP:HB2	1.63	0.78
1:B:3162:LEU:HD12	1:B:3166:GLN:HG2	1.66	0.78
1:A:1022:ASN:HD21	1:A:1024:GLU:HG2	1.48	0.77
1:A:1324:GLN:NE2	5:A:1453:NAP:H2A	1.98	0.77
1:A:1328:GLN:HE21	1:A:1361:ALA:CA	1.97	0.76
1:A:1158:MET:CE	1:A:1162:LEU:HB3	2.17	0.75
1:B:3053:ASP:HB2	1:B:3160:ALA:N	1.96	0.75
1:B:3322:TYR:HB3	1:B:3324:GLN:HE22	1.51	0.75
1:B:2760:ALA:HB3	1:B:2806:THR:OG1	1.87	0.75
1:B:2930:TRP:CE2	1:B:2934:VAL:HG21	2.21	0.74
1:A:1180:SER:OG	1:A:1262:GLN:NE2	2.20	0.74



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:3162:LEU:HD12	1:B:3166:GLN:CG	2.17	0.74
1:A:1078:ASN:N	1:A:1078:ASN:ND2	2.36	0.74
1:B:3367:THR:HG23	1:B:3372:LEU:O	1.87	0.74
1:A:876:ASN:C	1:A:876:ASN:HD22	1.91	0.74
1:B:2912:LEU:CD2	1:B:2934:VAL:HG22	2.17	0.74
1:A:959:SER:O	1:A:960:ASN:HB3	1.86	0.74
1:A:1324:GLN:HG2	1:A:1357:ASP:HB3	1.70	0.73
1:A:1022:ASN:HD22	1:A:1024:GLU:H	1.36	0.73
1:A:775:GLU:HG2	1:A:961:ASP:HB3	1.71	0.73
1:A:1071:THR:CG2	1:A:1072:ALA:H	2.00	0.73
1:B:3285:GLN:HG2	1:B:3287:LYS:HG2	1.71	0.73
1:A:965:LYS:HD2	1:A:968:LYS:HD2	1.68	0.72
1:B:3198:HIS:HB2	1:B:3202:GLY:HA2	1.71	0.72
1:B:2889:TYR:OH	1:B:3396:GLY:HA2	1.89	0.72
1:A:965:LYS:HG3	1:A:968:LYS:HB2	1.71	0.72
1:A:1243:PRO:HG3	1:A:1342:GLN:HE21	1.54	0.72
1:B:2966:ARG:HG3	1:B:2966:ARG:O	1.90	0.72
1:A:1062:LYS:HG3	1:A:1087:PRO:HG3	1.70	0.71
1:A:780:ALA:HB2	1:A:948:VAL:HG21	1.70	0.71
1:B:2765:LYS:NZ	1:B:2919:GLU:OE1	2.24	0.71
1:B:2959:SER:HA	1:B:3110:GLN:HE22	1.55	0.71
1:B:3019:THR:HG23	1:B:3025:LEU:CD1	2.20	0.71
1:A:816:GLU:HB2	1:A:1229:ARG:NH2	2.06	0.70
1:A:1127:VAL:HA	1:A:1130:LYS:HE3	1.73	0.70
1:A:962:ARG:O	1:A:963:SER:O	2.09	0.70
1:A:1036:PHE:HB2	1:A:1225:PRO:HB2	1.73	0.70
1:A:887:ARG:HG2	1:A:918:ASP:OD2	1.92	0.70
1:A:946:ASP:OD1	1:A:946:ASP:O	2.09	0.69
1:B:3111:GLN:O	1:B:3115:LEU:HD12	1.92	0.69
1:B:3053:ASP:CB	1:B:3160:ALA:H	1.97	0.69
1:A:799:GLU:HG2	1:A:802:VAL:HG22	1.74	0.69
1:A:1062:LYS:HE3	1:A:1087:PRO:CG	2.21	0.69
1:A:1198:HIS:NE2	1:A:1206:VAL:HG22	2.08	0.69
1:B:3107:LEU:O	1:B:3110:GLN:HG2	1.93	0.69
1:B:3345:HIS:CE1	1:B:3389:ARG:HG2	2.28	0.69
1:B:3130:LYS:O	1:B:3132:LEU:N	2.25	0.69
1:A:1158:MET:HE3	1:A:1162:LEU:HB3	1.74	0.69
1:B:2878:ARG:HH12	1:B:2941:VAL:HG13	1.58	0.69
1:B:3247:VAL:HG12	1:B:3280:VAL:HB	1.75	0.68
1:B:3351:ASP:HB2	1:B:3399:LEU:HG	1.74	0.68
1:A:1048:ILE:HD13	1:A:1057:ALA:CB	2.23	0.68



A + 1	<b>A t</b> and <b>D</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:3240:PRO:HG2	1:B:3241:GLN:HE21	1.57	0.68
1:A:1022:ASN:ND2	1:A:1024:GLU:HG2	2.07	0.68
1:B:3322:TYR:HB3	1:B:3324:GLN:NE2	2.07	0.68
1:A:779:HIS:CE1	1:A:951:GLU:OE2	2.47	0.68
1:B:2971:LEU:HD12	1:B:3055:PRO:HG2	1.75	0.68
1:A:1118:ASN:HB3	1:A:1121:GLU:HB3	1.76	0.67
1:A:976:GLU:OE2	1:B:2784:LYS:HD2	1.94	0.67
1:A:765:LYS:NZ	1:A:919:GLU:HG3	2.10	0.67
1:A:991:ARG:HG3	1:A:991:ARG:NH1	1.92	0.67
1:A:1161:THR:O	1:A:1165:THR:CG2	2.39	0.66
1:B:3314:ARG:O	1:B:3316:PRO:HD3	1.96	0.66
1:A:1158:MET:HE3	1:A:1159:PRO:HD2	1.76	0.66
1:A:912:LEU:HD12	1:A:934:VAL:HA	1.78	0.66
1:A:1238:ARG:O	1:A:1240:PRO:HD3	1.95	0.66
1:A:961:ASP:C	1:A:963:SER:H	1.99	0.66
1:A:848:VAL:HG12	1:A:848:VAL:O	1.94	0.66
1:A:1078:ASN:HD22	1:A:1078:ASN:H	1.44	0.66
1:A:1324:GLN:HE22	5:A:1453:NAP:C2A	2.07	0.66
1:B:3180:SER:OG	1:B:3262:GLN:NE2	2.30	0.65
1:B:2912:LEU:HD23	1:B:2934:VAL:HG22	1.78	0.65
1:A:1351:ASP:HB2	1:A:1399:LEU:HG	1.79	0.65
1:B:3193:ALA:HB2	1:B:3251:THR:HG21	1.79	0.65
1:B:2794:VAL:HG13	1:B:2795:HIS:HD2	1.62	0.65
1:B:2840:SER:HB2	1:B:3386:ASP:OD1	1.97	0.64
1:B:3242:VAL:HG11	1:B:3343:GLY:O	1.97	0.64
1:B:3158:MET:HE3	1:B:3162:LEU:HD23	1.78	0.64
1:B:2947:ASP:O	1:B:2949:ASN:N	2.30	0.64
1:B:2878:ARG:NH1	1:B:2941:VAL:HG13	2.13	0.64
1:B:2757:ILE:HG12	1:B:2803:LEU:HD12	1.80	0.64
1:A:1058:ASN:CG	1:A:1058:ASN:O	2.36	0.64
1:A:1268:GLN:HE21	1:A:1302:LYS:HD3	1.62	0.64
1:B:3283:CYS:HB2	1:B:3289:ASP:CB	2.27	0.64
1:B:3158:MET:HE3	1:B:3159:PRO:HD2	1.79	0.63
1:B:2946:ASP:OD2	1:B:2946:ASP:N	2.30	0.63
1:B:3019:THR:CG2	1:B:3025:LEU:HB2	2.28	0.63
1:A:1328:GLN:HE22	1:A:1364:ARG:HD2	1.61	0.63
1:A:1048:ILE:HD13	1:A:1057:ALA:HB1	1.79	0.63
1:A:1069:ARG:HG2	1:A:1070:ASN:N	2.12	0.63
1:A:1322:TYR:HB3	1:A:1324:GLN:NE2	2.13	0.63
1:B:3158:MET:CE	1:B:3162:LEU:HB3	2.29	0.63
1:B:3242:VAL:HG13	1:B:3243:PRO:HD2	1.80	0.63



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:3195:VAL:HA	6:B:6093:HOH:O	1.99	0.63
1:B:3363:GLN:HE21	1:B:3378:GLY:CA	2.12	0.62
1:B:2915:ARG:HD2	1:B:2930:TRP:HB2	1.79	0.62
1:B:2905:GLU:O	1:B:2906:LEU:HD23	1.99	0.62
1:B:2884:LEU:N	1:B:2884:LEU:HD12	2.14	0.62
1:B:3286:SER:HB3	1:B:3312:TYR:CZ	2.34	0.62
1:A:1283:CYS:HB2	1:A:1289:ASP:HB3	1.82	0.62
1:B:2774:CYS:O	1:B:2778:LYS:HG2	2.00	0.62
1:B:2971:LEU:CD1	1:B:3055:PRO:HG2	2.29	0.62
1:B:3312:TYR:H	1:B:3321:LYS:HE3	1.64	0.62
1:B:3165:THR:OG1	1:B:3166:GLN:NE2	2.30	0.61
1:A:991:ARG:CG	1:A:991:ARG:NH1	2.55	0.61
1:B:3002:ASN:HB3	6:B:6013:HOH:O	2.00	0.61
1:B:2840:SER:HB2	1:B:3386:ASP:CG	2.21	0.61
1:A:987:VAL:CG2	1:A:1086:PRO:HD3	2.31	0.61
1:B:2878:ARG:NH1	1:B:2941:VAL:CG1	2.64	0.61
1:A:1022:ASN:HD21	1:A:1024:GLU:CG	2.14	0.60
1:B:2760:ALA:HB1	1:B:2815:PRO:HG3	1.82	0.60
1:B:2974:VAL:HG12	1:B:2976:GLU:H	1.67	0.60
1:A:1402:TYR:O	1:A:1406:ASN:HB2	2.02	0.60
5:B:2453:NAP:H1D	6:B:6095:HOH:O	2.01	0.60
1:A:1057:ALA:HA	1:A:1090:ILE:HD11	1.83	0.60
1:A:1162:LEU:HD12	1:A:1166:GLN:HG2	1.84	0.59
1:B:3193:ALA:CB	5:B:2453:NAP:H51N	2.30	0.59
1:B:3353:THR:HG22	5:B:2453:NAP:N6A	2.16	0.59
1:B:2912:LEU:HD22	1:B:2934:VAL:HG22	1.82	0.59
1:A:1239:ASN:HD22	1:A:1239:ASN:C	2.06	0.59
1:A:1373:SER:C	1:A:1375:GLU:H	2.05	0.59
1:A:1123:GLN:O	1:A:1127:VAL:HG23	2.02	0.59
1:B:2828:MET:SD	1:B:2906:LEU:HD13	2.43	0.59
1:B:2973:TYR:HE2	1:B:3059:HIS:CD2	2.21	0.59
1:A:1361:ALA:O	1:A:1365:ILE:HG13	2.02	0.58
1:B:3161:THR:O	1:B:3165:THR:HG23	2.03	0.58
1:B:2757:ILE:CG1	1:B:2803:LEU:HD12	2.34	0.58
1:A:1268:GLN:NE2	1:A:1302:LYS:HD3	2.17	0.58
1:B:2842:LYS:HD3	1:B:2846:ASN:ND2	2.16	0.58
1:B:3019:THR:O	1:B:3022:ASN:HB2	2.03	0.58
1:B:2973:TYR:HE2	1:B:3059:HIS:HD2	1.52	0.58
1:B:3247:VAL:HG23	1:B:3348:VAL:HA	1.85	0.58
1:A:924:GLU:HG3	1:A:1106:PRO:HD2	1.85	0.58
1:B:3324:GLN:NE2	5:B:2453:NAP:H2A	2.18	0.58



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:B:3033:LEU:HD22	1:B:3188:VAL:HG11	1.85	0.58	
1:A:1266:ASP:HB3	1:A:1272:MET:HG3	1.86	0.58	
1:B:3262:GLN:O	1:B:3266:ASP:OD2	2.22	0.57	
1:A:779:HIS:ND1	1:A:951:GLU:OE2	2.37	0.57	
1:A:876:ASN:O	1:A:876:ASN:ND2	2.27	0.57	
1:A:964:TRP:CG	1:A:1162:LEU:HD13	2.39	0.57	
1:B:3337:ARG:HG3	1:B:3341:GLU:OE1	2.05	0.57	
1:B:3052:GLU:HB3	1:B:3158:MET:O	2.04	0.57	
1:A:765:LYS:HZ3	1:A:919:GLU:HG3	1.69	0.57	
1:A:1367:THR:HG23	1:A:1372:LEU:O	2.04	0.57	
1:B:2981:THR:HG21	1:B:2994:ALA:HB2	1.86	0.57	
1:B:2793:ILE:O	1:B:2793:ILE:HG13	2.04	0.57	
1:B:3360:LYS:CB	1:B:3364:ARG:NH1	2.64	0.57	
1:A:971:LEU:CD2	1:A:1063:VAL:HG22	2.35	0.57	
1:B:3287:LYS:NZ	1:B:3315:GLU:OE1	2.36	0.57	
1:B:3363:GLN:HE21	1:B:3378:GLY:HA3	1.68	0.57	
1:A:767:GLN:O	1:A:771:LYS:HG2	2.05	0.57	
1:A:887:ARG:CG	1:A:918:ASP:OD2	2.53	0.57	
1:A:1257:ARG:NE	1:A:1295:GLU:OE1	2.38	0.57	
1:B:2821:PHE:HE1	1:B:2825:LEU:HD11	1.68	0.57	
1:A:775:GLU:HG2	1:A:961:ASP:HB2	1.83	0.56	
1:B:2912:LEU:HD21	1:B:2915:ARG:HH12	1.68	0.56	
1:A:1057:ALA:HA	1:A:1090:ILE:CG1	2.35	0.56	
1:B:2976:GLU:O	1:B:2976:GLU:HG2	2.05	0.56	
1:B:2895:PHE:O	1:B:2899:VAL:HG23	2.05	0.56	
1:B:2939:CYS:HA	6:B:6058:HOH:O	2.05	0.56	
1:B:3133:GLN:O	1:B:3137:GLU:HG3	2.05	0.56	
1:B:3180:SER:H	1:B:3261:GLN:NE2	2.03	0.56	
1:A:1410:SER:O	1:A:1412:SER:N	2.39	0.56	
1:B:2930:TRP:NE1	1:B:2934:VAL:HG21	2.21	0.56	
1:B:2964:TRP:CZ2	1:B:2966:ARG:HD2	2.41	0.56	
1:B:2766:SER:OG	1:B:2884:LEU:HD22	2.05	0.56	
1:A:981:THR:HG21	1:A:994:ALA:HB2	1.86	0.56	
1:A:1322:TYR:HB3	1:A:1324:GLN:HE22	1.71	0.56	
1:B:2794:VAL:HG13	1:B:2795:HIS:CD2	2.39	0.56	
1:B:2979:ASP:OD1	1:B:2980:LEU:N	2.38	0.56	
1:B:3257:ARG:O	1:B:3261:GLN:HG3	2.05	0.56	
1:B:3353:THR:CG2	5:B:2453:NAP:H62A	2.18	0.56	
1:A:965:LYS:HG3	1:A:968:LYS:CB	2.36	0.55	
1:B:3000:ARG:HA	1:B:3014:PHE:O	2.07	0.55	
1:A:1333:GLU:HA	1:A:1369:GLN:NE2	2.21	0.55	



A + a 1		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:B:2773:LEU:O	1:B:2776:ILE:HG22	2.06	0.55	
1:B:2846:ASN:O	1:B:3385:ARG:NH2	2.40	0.55	
1:B:3110:GLN:HG3	1:B:3111:GLN:N	2.22	0.55	
1:A:799:GLU:HG2	1:A:802:VAL:CG2	2.36	0.55	
1:A:1371:LYS:CG	1:A:1371:LYS:O	2.55	0.55	
1:A:1346:ILE:HD13	1:A:1362:ILE:CD1	2.37	0.55	
1:B:2760:ALA:HB1	1:B:2815:PRO:CG	2.37	0.55	
1:A:1057:ALA:HA	1:A:1090:ILE:HG12	1.89	0.55	
1:A:1194:ILE:O	5:A:1453:NAP:H5N	2.07	0.55	
1:A:1316:PRO:HG2	1:A:1317:ASP:OD1	2.05	0.55	
1:B:2757:ILE:HG12	1:B:2803:LEU:HB2	1.89	0.55	
1:B:3110:GLN:O	1:B:3113:ALA:HB3	2.07	0.55	
1:A:1051:LEU:HD21	1:A:1163:LEU:HD12	1.89	0.54	
1:A:1056:PRO:C	1:A:1058:ASN:H	2.11	0.54	
1:A:1193:ALA:HB1	5:A:1453:NAP:H51N	1.89	0.54	
1:B:2877:VAL:HG12	1:B:2878:ARG:O	2.06	0.54	
1:A:1239:ASN:ND2	1:A:1241:GLN:H	2.06	0.54	
1:A:762:GLU:HB2	1:A:809:PHE:CE1	2.43	0.54	
1:A:959:SER:O	1:A:960:ASN:CB	2.54	0.54	
1:B:3325:ASP:O	1:B:3329:GLU:HB2	2.08	0.54	
1:A:1056:PRO:O	1:A:1058:ASN:N	2.38	0.54	
1:A:1318:ARG:CB	1:A:1319:PRO:HD2	2.38	0.54	
1:B:3306:ARG:C	1:B:3307:GLU:HG2	2.28	0.54	
1:A:756:THR:OG1	1:A:799:GLU:OE2	2.25	0.54	
1:A:1036:PHE:CE1	1:A:1172:PRO:HB3	2.43	0.54	
1:B:2970:ARG:HB3	1:B:3079:TRP:CZ3	2.43	0.54	
1:B:2964:TRP:HZ2	1:B:2966:ARG:NH1	2.06	0.53	
1:B:2843:VAL:HG22	1:B:3382:SER:OG	2.09	0.53	
1:B:3351:ASP:OD1	1:B:3353:THR:HB	2.07	0.53	
1:A:1048:ILE:HD13	1:A:1057:ALA:HB2	1.91	0.53	
1:A:1057:ALA:HA	1:A:1090:ILE:CD1	2.38	0.53	
1:B:2787:SER:HB2	1:B:2789:GLU:HG2	1.90	0.53	
1:B:2802:VAL:O	1:B:2879:PHE:HA	2.08	0.53	
1:B:3010:ARG:HE	5:B:2453:NAP:C5N	2.22	0.53	
1:B:3132:LEU:O	1:B:3134:GLU:N	2.41	0.53	
1:A:912:LEU:HD22	1:A:915:ARG:NH1	2.16	0.53	
1:A:1346:ILE:HD13	1:A:1362:ILE:HD13	1.89	0.53	
1:B:3408:LEU:HA	1:B:3411:GLU:HB2	1.91	0.53	
1:A:1004:GLN:NE2	1:A:1008:SER:OG	2.42	0.53	
1:A:775:GLU:CD	1:A:961:ASP:HB2	2.29	0.53	
1:B:3345:HIS:ND1	1:B:3389:ARG:HA	2.23	0.53	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:1394:ILE:HG22	1:A:1396:GLY:H	1.73	0.52	
1:B:3054:ALA:O	1:B:3056:PRO:HD3	2.09	0.52	
1:A:846:ASN:O	1:A:1385:ARG:NH2	2.42	0.52	
1:A:1127:VAL:HA	1:A:1130:LYS:CE	2.38	0.52	
1:A:1410:SER:O	1:A:1413:ILE:HG22	2.08	0.52	
1:B:2752:ARG:HD2	1:B:2782:ASP:HB2	1.91	0.52	
1:B:3309:TYR:CD2	1:B:3331:LEU:HD11	2.45	0.52	
1:B:2840:SER:O	1:B:2843:VAL:HB	2.09	0.52	
1:B:3019:THR:HG21	1:B:3025:LEU:HB2	1.89	0.52	
1:B:2966:ARG:O	1:B:2966:ARG:CG	2.57	0.52	
1:A:1328:GLN:HE22	1:A:1364:ARG:NH1	2.08	0.52	
1:B:3245:ILE:HD13	1:B:3335:VAL:HG22	1.91	0.52	
1:B:3363:GLN:HA	1:B:3381:ILE:HD11	1.92	0.52	
1:A:970:ARG:HB3	1:A:1079:TRP:CZ3	2.44	0.52	
1:A:1286:SER:HA	1:A:1312:TYR:CE2	2.44	0.52	
1:B:3162:LEU:HD12	1:B:3166:GLN:HG3	1.90	0.52	
1:B:3242:VAL:CG1	1:B:3344:GLY:HA2	2.38	0.52	
1:A:1162:LEU:HD12	1:A:1166:GLN:CG	2.40	0.51	
1:B:3313:SER:O	1:B:3320:LYS:HE3	2.10	0.51	
1:A:974:VAL:HG12	1:A:976:GLU:H	1.76	0.51	
1:A:1373:SER:C	1:A:1375:GLU:N	2.63	0.51	
1:B:3034:GLY:O	1:B:3226:CYS:HA	2.10	0.51	
1:B:2972:THR:HG21	1:B:3064:GLU:OE2	2.10	0.51	
1:A:1087:PRO:O	1:A:1088:CYS:HB3	2.10	0.51	
1:A:1143:ASN:O	1:A:1207:HIS:HE1	1.94	0.51	
1:B:3019:THR:HG23	1:B:3025:LEU:HB2	1.93	0.51	
1:B:3158:MET:CE	1:B:3159:PRO:HD2	2.41	0.51	
1:B:3162:LEU:CD1	1:B:3166:GLN:HG3	2.41	0.51	
1:B:3309:TYR:HB3	1:B:3326:VAL:HG11	1.92	0.51	
1:A:775:GLU:CG	1:A:961:ASP:HB2	2.41	0.51	
1:A:1360:LYS:O	1:A:1364:ARG:HG3	2.11	0.51	
1:B:3158:MET:HE3	1:B:3162:LEU:HB3	1.92	0.51	
1:B:3330:GLN:C	1:B:3331:LEU:HD12	2.31	0.51	
1:A:1064:GLU:HA	1:A:1080:LYS:O	2.11	0.51	
1:A:1318:ARG:HB2	1:A:1319:PRO:HD2	1.92	0.51	
1:B:2821:PHE:CE1	1:B:2825:LEU:HD11	2.45	0.51	
1:A:1058:ASN:HA	1:A:1089:THR:HB	1.93	0.50	
1:A:1157:GLN:O	1:A:1159:PRO:HD3	2.10	0.50	
1:A:1239:ASN:HD22	1:A:1240:PRO:N	2.08	0.50	
1:B:3180:SER:H	1:B:3261:GLN:HE21	1.58	0.50	
1:A:964:TRP:CH2	1:A:966:ARG:HG3	2.46	0.50	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:1071:THR:CG2	1:A:1072:ALA:N	2.59	0.50	
1:A:1195:VAL:HA	5:A:1453:NAP:C5N	2.41	0.50	
1:A:904:GLU:OE2	1:A:910:ARG:NH1	2.42	0.50	
1:B:3015:VAL:O	1:B:3189:HIS:HA	2.12	0.50	
1:A:1268:GLN:NE2	1:A:1302:LYS:HE2	2.26	0.50	
1:B:3351:ASP:OD1	1:B:3353:THR:N	2.43	0.50	
1:B:3076:ILE:HG23	1:B:3076:ILE:O	2.11	0.50	
1:B:3360:LYS:HE2	1:B:3360:LYS:HA	1.94	0.50	
1:B:3240:PRO:HG2	1:B:3241:GLN:NE2	2.26	0.50	
1:A:961:ASP:C	1:A:963:SER:N	2.65	0.49	
1:A:1239:ASN:C	1:A:1239:ASN:ND2	2.64	0.49	
1:A:898:ALA:O	1:A:902:LEU:HG	2.12	0.49	
1:A:979:ASP:OD1	1:A:979:ASP:C	2.50	0.49	
1:A:1140:TRP:CD1	1:A:1409:ARG:HD2	2.47	0.49	
1:B:2790:GLU:HG2	1:B:2790:GLU:O	2.12	0.49	
1:B:3004:GLN:NE2	1:B:3008:SER:OG	2.46	0.49	
1:B:3145:THR:O	1:B:3149:VAL:HG23	2.12	0.49	
1:A:910:ARG:HD3	1:A:913:LYS:HA	1.95	0.49	
1:A:971:LEU:HD23	1:A:1063:VAL:HG22	1.95	0.49	
1:A:1022:ASN:ND2	1:A:1024:GLU:CG	2.73	0.49	
1:A:1198:HIS:NE2	1:A:1206:VAL:CG2	2.75	0.49	
1:B:2879:PHE:CD1	1:B:2903:LEU:HD13	2.47	0.49	
1:B:2959:SER:HA	1:B:3110:GLN:NE2	2.24	0.49	
1:A:837:GLU:O	1:A:838:ARG:CB	2.61	0.49	
1:A:1158:MET:HE3	1:A:1162:LEU:HD23	1.94	0.49	
1:A:1309:TYR:HB3	1:A:1326:VAL:HG11	1.95	0.49	
1:B:2968:LYS:O	1:B:3065:MET:HA	2.13	0.49	
1:A:912:LEU:CD1	1:A:934:VAL:HA	2.42	0.49	
1:B:3140:TRP:HA	1:B:3140:TRP:CE3	2.47	0.49	
1:B:3069:ARG:HG2	6:B:6069:HOH:O	2.12	0.48	
1:B:3010:ARG:NH2	5:B:2453:NAP:H51N	2.28	0.48	
1:B:3123:GLN:NE2	1:B:3126:LEU:HD12	2.28	0.48	
1:B:2759:TYR:HA	1:B:2805:VAL:O	2.12	0.48	
1:B:3144:PRO:HA	1:B:3148:GLU:OE1	2.13	0.48	
1:A:1346:ILE:CD1	1:A:1362:ILE:HD11	2.43	0.48	
1:B:2964:TRP:HZ2	1:B:2966:ARG:HH11	1.59	0.48	
1:A:843:VAL:O	1:A:847:SER:HB2	2.14	0.48	
1:B:3122:LYS:O	1:B:3126:LEU:HG	2.13	0.48	
1:B:3089:THR:OG1	1:B:3092:GLN:HG3	2.13	0.48	
1:A:761:THR:HB	1:A:766:SER:HB2	1.95	0.48	
1:A:977:ALA:HB2	1:A:1060:VAL:CG2	2.44	0.48	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:1328:GLN:HE22	1:A:1364:ARG:HH11	1.61	0.48	
1:A:784:LYS:HD2	1:A:784:LYS:HA	1.59	0.48	
1:A:996:ARG:O	1:A:1017:LEU:HA	2.14	0.48	
1:B:3299:ALA:O	1:B:3304:VAL:HB	2.13	0.48	
1:B:3247:VAL:HG11	1:B:3327:LEU:HD21	1.96	0.47	
1:B:3324:GLN:HE22	5:B:2453:NAP:H2A	1.79	0.47	
1:A:1105:THR:OG1	1:A:1108:GLN:HG3	2.13	0.47	
1:A:1158:MET:CE	1:A:1159:PRO:HD2	2.44	0.47	
1:B:3053:ASP:HB3	1:B:3160:ALA:CB	2.45	0.47	
1:A:1110:GLN:HE21	1:A:1110:GLN:HA	1.78	0.47	
1:B:3057:ALA:HA	1:B:3090:ILE:HG22	1.96	0.47	
1:B:3140:TRP:HA	1:B:3140:TRP:HE3	1.80	0.47	
1:B:3377:ALA:O	1:B:3381:ILE:HG13	2.15	0.47	
1:A:1224:VAL:O	1:A:1224:VAL:HG12	2.14	0.47	
1:A:1268:GLN:HE22	1:A:1302:LYS:HE2	1.80	0.47	
1:B:3351:ASP:CB	1:B:3399:LEU:HG	2.44	0.47	
1:A:947:ASP:OD1	1:A:947:ASP:N	2.48	0.47	
1:A:1049:GLU:HG3	1:A:1049:GLU:O	2.15	0.47	
1:A:1333:GLU:HA	1:A:1369:GLN:HE21	1.78	0.47	
1:A:876:ASN:C	1:A:876:ASN:ND2	2.64	0.46	
1:B:2970:ARG:HD2	1:B:3079:TRP:CE3	2.49	0.46	
1:B:3379:VAL:O	1:B:3382:SER:HB3	2.15	0.46	
1:B:2760:ALA:HB2	1:B:2788:MET:SD	2.55	0.46	
1:A:964:TRP:CB	1:A:1162:LEU:HD13	2.45	0.46	
1:B:3362:ILE:O	1:B:3366:MET:HG2	2.15	0.46	
1:B:3405:THR:O	1:B:3409:ARG:HG3	2.15	0.46	
1:A:772:THR:O	1:A:776:ILE:HG13	2.15	0.46	
1:A:1027:TYR:CE2	1:A:1188:VAL:HG22	2.49	0.46	
1:B:3400:ARG:O	1:B:3404:VAL:HB	2.16	0.46	
1:A:1062:LYS:CG	1:A:1087:PRO:HG3	2.42	0.46	
1:B:2842:LYS:HA	1:B:2846:ASN:HD22	1.80	0.46	
1:A:780:ALA:CB	1:A:948:VAL:HG21	2.42	0.46	
1:A:1059:HIS:O	1:A:1061:VAL:HG13	2.16	0.46	
1:B:2902:LEU:HD23	1:B:2905:GLU:OE1	2.16	0.46	
1:B:2788:MET:HE3	1:B:2821:PHE:CD1	2.51	0.46	
1:B:2971:LEU:HD12	1:B:3055:PRO:CG	2.44	0.46	
1:A:1049:GLU:O	1:A:1049:GLU:CG	2.64	0.46	
1:B:2787:SER:CB	1:B:2789:GLU:HG2	2.46	0.46	
1:B:2884:LEU:N	1:B:2884:LEU:CD1	2.77	0.46	
1:B:2889:TYR:CD1	1:B:3352:VAL:HG21	2.50	0.46	
1:A:799:GLU:O	1:A:877:VAL:HG22	2.16	0.46	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:1362:ILE:O	1:A:1366:MET:HG2	2.16	0.46	
1:B:2846:ASN:O	1:B:2891:HIS:CE1	2.69	0.46	
1:B:3281:PHE:CG	1:B:3282:GLY:N	2.84	0.46	
1:A:1080:LYS:NZ	1:B:3079:TRP:O	2.48	0.45	
1:B:3104:PRO:HG3	1:B:3146:MET:SD	2.56	0.45	
1:A:1317:ASP:OD1	1:A:1317:ASP:N	2.46	0.45	
1:B:2775:GLU:OE1	1:B:2775:GLU:HA	2.17	0.45	
1:A:961:ASP:O	1:A:963:SER:N	2.48	0.45	
1:A:1309:TYR:CE1	1:A:1331:LEU:HD21	2.51	0.45	
1:B:2776:ILE:HG23	1:B:2777:PHE:N	2.32	0.45	
1:B:2904:GLU:OE1	1:B:2910:ARG:NH2	2.49	0.45	
1:B:3312:TYR:H	1:B:3321:LYS:HG3	1.82	0.45	
1:A:762:GLU:HG3	1:A:809:PHE:CG	2.51	0.45	
1:B:2755:ALA:HB2	1:B:2801:LEU:HD23	1.98	0.45	
1:B:3132:LEU:O	1:B:3133:GLN:C	2.55	0.45	
1:A:1372:LEU:HB3	1:A:1376:ASP:CB	2.41	0.45	
1:B:2786:MET:SD	1:B:2791:TYR:HB2	2.57	0.45	
1:B:3113:ALA:C	1:B:3115:LEU:H	2.19	0.45	
1:A:840:SER:O	1:A:844:ARG:HG3	2.17	0.45	
1:A:1055:PRO:O	1:A:1056:PRO:C	2.55	0.45	
1:B:3026:GLN:HA	1:B:3026:GLN:OE1	2.17	0.45	
1:B:3247:VAL:CG2	1:B:3348:VAL:HG22	2.47	0.45	
1:B:3338:ALA:HA	1:B:3342:GLN:HB2	1.99	0.45	
1:A:787:SER:OG	1:A:789:GLU:HG2	2.16	0.45	
1:B:3380:PHE:CD1	1:B:3380:PHE:C	2.90	0.45	
1:B:3112:PHE:HZ	1:B:3146:MET:HE3	1.82	0.44	
1:A:875:ALA:HA	1:A:907:GLY:O	2.16	0.44	
1:B:2806:THR:O	1:B:2883:GLY:HA2	2.18	0.44	
1:B:3306:ARG:O	1:B:3307:GLU:HG2	2.18	0.44	
1:A:841:TYR:HE2	1:A:846:ASN:ND2	2.16	0.44	
1:B:3019:THR:HG22	1:B:3022:ASN:HB2	1.99	0.44	
1:B:3067:GLU:OE1	1:B:3080:LYS:HG3	2.16	0.44	
1:A:1050:ARG:HD2	1:A:1050:ARG:O	2.17	0.44	
1:A:1061:VAL:HG23	1:A:1061:VAL:O	2.18	0.44	
1:A:1351:ASP:CB	1:A:1399:LEU:HG	2.47	0.44	
5:A:1453:NAP:O3D	5:A:1453:NAP:PA	2.70	0.44	
1:B:2769:TYR:CD2	1:B:2884:LEU:HD21	2.52	0.44	
1:B:2961:ASP:C	1:B:2963:SER:H	2.21	0.44	
1:B:2971:LEU:CD2	1:B:3063:VAL:HG22	2.48	0.44	
1:B:3062:LYS:HD2	1:B:3081:ASP:OD1	2.18	0.44	
1:B:3360:LYS:HB3	1:B:3364:ARG:CZ	2.44	0.44	



	<b>A t</b> area <b>D</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:830:HIS:NE2	1:A:838:ARG:O	2.34	0.44
1:A:1080:LYS:NZ	1:B:3080:LYS:HA	2.33	0.44
1:A:1080:LYS:HZ2	1:B:3080:LYS:HA	1.82	0.44
1:B:3053:ASP:HB3	1:B:3160:ALA:HB2	1.99	0.44
1:B:3134:GLU:OE1	1:B:3134:GLU:HA	2.18	0.44
1:B:3201:ASP:HB2	1:B:3402:TYR:OH	2.18	0.44
1:B:3330:GLN:HB2	1:B:3331:LEU:HD12	1.98	0.44
1:B:3115:LEU:HD22	1:B:3157:GLN:O	2.18	0.44
1:B:3132:LEU:O	1:B:3135:TYR:N	2.50	0.44
1:A:841:TYR:CE2	1:A:846:ASN:ND2	2.86	0.43
1:A:1089:THR:HG23	1:A:1092:GLN:OE1	2.18	0.43
1:A:1249:PRO:HG3	1:A:1354:MET:HG3	2.00	0.43
1:B:2928:ARG:HH12	1:B:3130:LYS:HA	1.82	0.43
1:B:3193:ALA:CB	5:B:2453:NAP:C5D	2.95	0.43
1:B:3359:LEU:HD23	1:B:3359:LEU:C	2.38	0.43
1:A:1027:TYR:CE1	1:A:1177:ILE:HG21	2.53	0.43
1:A:1331:LEU:O	1:A:1332:ALA:C	2.56	0.43
1:A:1142:LYS:O	1:A:1143:ASN:C	2.56	0.43
1:B:3110:GLN:CG	1:B:3111:GLN:N	2.81	0.43
1:B:3078:ASN:HB2	1:B:3080:LYS:HZ3	1.82	0.43
1:A:889:TYR:CD1	1:A:1352:VAL:HG21	2.54	0.43
1:A:1132:LEU:O	1:A:1136:GLU:HG2	2.18	0.43
1:B:2882:PHE:CD1	1:B:2915:ARG:HB3	2.53	0.43
1:A:813:ASP:HB3	1:A:814:PRO:CD	2.49	0.43
1:B:3242:VAL:CG1	1:B:3343:GLY:O	2.65	0.43
1:B:3250:GLY:O	1:B:3253:ILE:HG22	2.18	0.43
1:B:2845:PHE:CE2	1:B:2898:ALA:HA	2.54	0.43
1:A:1158:MET:HA	1:A:1159:PRO:HD3	1.81	0.43
1:A:1242:VAL:HG22	1:A:1243:PRO:HD2	2.00	0.43
1:B:3158:MET:HE2	1:B:3159:PRO:O	2.18	0.43
1:A:779:HIS:HB3	1:A:948:VAL:HG22	2.01	0.43
1:A:961:ASP:CG	1:A:962:ARG:N	2.72	0.43
1:B:3103:PRO:HA	1:B:3104:PRO:HD3	1.93	0.43
1:B:2877:VAL:HG12	1:B:2878:ARG:N	2.34	0.42
1:B:3220:ALA:O	1:B:3221:ASP:HB2	2.19	0.42
1:A:1056:PRO:C	1:A:1058:ASN:N	2.72	0.42
1:A:1385:ARG:HG2	1:A:1390:TYR:HB3	2.00	0.42
1:B:2912:LEU:HD23	1:B:2930:TRP:CD1	2.55	0.42
1:A:1039:ASN:O	1:A:1095:LYS:HD2	2.19	0.42
1:A:1113:ALA:C	1:A:1115:LEU:H	2.22	0.42
1:B:3019:THR:HG22	1:B:3022:ASN:CB	2.48	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:1134:GLU:CD	1:A:1134:GLU:H	2.23	0.42
1:A:1143:ASN:N	1:A:1144:PRO:CD	2.82	0.42
1:B:3003:LEU:HD21	1:B:3014:PHE:HB2	2.02	0.42
1:A:1343:GLY:HA2	1:A:1389:ARG:NH2	2.34	0.42
1:B:2912:LEU:HD23	1:B:2934:VAL:CG2	2.47	0.42
1:B:3214:TRP:O	1:B:3218:ILE:HG23	2.18	0.42
1:A:762:GLU:HG3	1:A:809:PHE:CD1	2.55	0.42
1:A:936:LYS:HA	1:A:936:LYS:HD2	1.86	0.42
1:B:2789:GLU:C	1:B:2791:TYR:H	2.23	0.42
1:B:2823:CYS:HA	1:B:2826:MET:HB2	2.02	0.42
1:B:3050:ARG:O	1:B:3050:ARG:HG3	2.18	0.42
1:B:3130:LYS:O	1:B:3132:LEU:HG	2.19	0.42
1:A:1195:VAL:HA	5:A:1453:NAP:H5N	2.01	0.42
1:B:3121:GLU:O	1:B:3125:LEU:HG	2.20	0.42
1:B:3401:THR:O	1:B:3405:THR:HB	2.20	0.42
1:A:904:GLU:OE2	1:A:910:ARG:NH2	2.50	0.42
1:A:985:SER:HA	1:A:990:LYS:O	2.19	0.42
1:B:3309:TYR:CE1	1:B:3331:LEU:HD21	2.55	0.42
1:B:3409:ARG:O	1:B:3413:ILE:HG13	2.19	0.42
1:A:965:LYS:CD	1:A:968:LYS:HD2	2.43	0.42
1:B:3244:CYS:HA	1:B:3345:HIS:O	2.19	0.42
1:A:970:ARG:HD2	1:A:1079:TRP:CE3	2.55	0.41
1:A:784:LYS:HG2	1:B:2976:GLU:OE1	2.21	0.41
1:A:901:THR:O	1:A:905:GLU:HG3	2.20	0.41
1:B:2779:HIS:HB2	1:B:2935:PHE:HZ	1.86	0.41
1:B:3257:ARG:HA	1:B:3260:TRP:CD2	2.55	0.41
1:A:970:ARG:HD3	1:A:972:THR:CG2	2.50	0.41
1:A:1062:LYS:CE	1:A:1087:PRO:HG3	2.42	0.41
1:A:1133:GLN:O	1:A:1134:GLU:C	2.57	0.41
1:B:2936:LYS:HE3	1:B:2940:ASP:OD2	2.21	0.41
1:B:2964:TRP:CG	1:B:3162:LEU:HD13	2.55	0.41
1:B:3162:LEU:O	1:B:3166:GLN:HG2	2.19	0.41
1:A:998:LEU:HD21	1:A:1018:HIS:HB2	2.01	0.41
1:A:1318:ARG:CB	1:A:1319:PRO:CD	2.98	0.41
1:B:3146:MET:HE2	1:B:3167:LEU:HD21	2.01	0.41
1:A:996:ARG:HG3	6:A:5035:HOH:O	2.19	0.41
1:A:1054:ALA:HB2	1:A:1160:ALA:HB2	2.01	0.41
1:B:3040:HIS:O	1:B:3044:VAL:HG23	2.20	0.41
1:B:3109:LEU:O	1:B:3112:PHE:N	2.54	0.41
1:B:3371:LYS:HA	1:B:3371:LYS:HD3	1.62	0.41
1:A:810:GLY:HA2	6:A:5051:HOH:O	2.20	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:2912:LEU:CD2	1:B:2934:VAL:CG2	2.94	0.41
1:A:1198:HIS:CE1	1:A:1206:VAL:HG22	2.54	0.41
1:A:1268:GLN:NE2	1:A:1302:LYS:CD	2.84	0.41
1:A:1324:GLN:CG	1:A:1357:ASP:HB3	2.45	0.41
1:B:2828:MET:HG2	1:B:2906:LEU:HD22	2.01	0.41
1:A:780:ALA:N	1:A:948:VAL:HG21	2.35	0.41
1:A:935:PHE:CE2	1:A:948:VAL:HG11	2.56	0.41
1:A:979:ASP:OD1	1:A:980:LEU:N	2.54	0.41
1:A:1263:ARG:HA	1:A:1263:ARG:HD3	1.81	0.41
1:B:2788:MET:HE2	1:B:2821:PHE:HB3	2.02	0.41
1:B:2793:ILE:HD13	1:B:2824:ALA:CB	2.51	0.41
1:B:2843:VAL:HG12	1:B:2844:ARG:N	2.36	0.41
1:B:3353:THR:CG2	5:B:2453:NAP:N6A	2.80	0.41
1:B:2773:LEU:O	1:B:2776:ILE:CG2	2.69	0.41
1:B:3158:MET:HA	1:B:3159:PRO:HD3	1.85	0.41
1:B:3347:TYR:CZ	1:B:3391:HIS:CD2	3.09	0.41
1:A:762:GLU:HG2	1:A:815:PRO:HB3	2.04	0.40
1:A:1013:ILE:HD13	1:A:1194:ILE:HD11	2.04	0.40
1:B:2928:ARG:O	1:B:2931:ALA:HB3	2.21	0.40
1:B:3109:LEU:O	1:B:3110:GLN:C	2.60	0.40
1:A:946:ASP:OD1	1:A:946:ASP:C	2.60	0.40
1:A:982:GLN:HA	1:A:982:GLN:OE1	2.20	0.40
1:A:1183:MET:HG2	1:A:1184:TYR:CE2	2.56	0.40
1:B:3266:ASP:HB3	1:B:3272:MET:HG3	2.02	0.40
1:B:3332:ALA:HB1	1:B:3365:ILE:HG23	2.02	0.40
1:A:1024:GLU:OE1	1:A:1024:GLU:HA	2.22	0.40
1:A:1317:ASP:C	1:A:1318:ARG:HG2	2.42	0.40
1:A:1328:GLN:HE21	1:A:1361:ALA:CB	2.31	0.40
1:B:2998:LEU:HD23	1:B:2998:LEU:HA	1.90	0.40
1:A:935:PHE:CZ	1:A:948:VAL:HG11	2.57	0.40
1:A:983:GLY:O	1:A:987:VAL:HG23	2.22	0.40
1:B:2756:THR:HG22	1:B:2758:LEU:HG	2.03	0.40
1:B:3055:PRO:O	1:B:3056:PRO:C	2.60	0.40
1:B:3062:LYS:HD2	1:B:3081:ASP:CG	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:GLN:OE1	$1:B:3364:ARG:NE[1_654]$	2.08	0.12



### 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	А	622/688~(90%)	569~(92%)	40 (6%)	13 (2%)	7 5
1	В	608/688~(88%)	548 (90%)	51 (8%)	9(2%)	10 10
All	All	1230/1376~(89%)	1117 (91%)	91 (7%)	22~(2%)	8 7

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	839	LYS
1	А	848	VAL
1	А	960	ASN
1	А	963	SER
1	А	1411	GLU
1	В	2948	VAL
1	В	3131	GLY
1	В	3133	GLN
1	А	838	ARG
1	А	962	ARG
1	А	1410	SER
1	В	2843	VAL
1	А	1370	GLY
1	В	3053	ASP
1	В	3114	SER
1	В	3286	SER
1	В	3374	GLU
1	А	1057	ALA
1	А	1069	ARG
1	В	3317	ASP
1	А	1055	PRO
1	А	978	PRO



#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Analysed Rotameric Outliers		Percentiles		
1	А	543/601~(90%)	506~(93%)	37~(7%)	16 21		
1	В	531/601~(88%)	496 (93%)	35~(7%)	16 22		
All	All	1074/1202~(89%)	1002~(93%)	72 (7%)	16 21		

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	751	LYS
1	А	752	ARG
1	А	787	SER
1	А	809	PHE
1	А	820	LYS
1	А	830	HIS
1	А	844	ARG
1	А	847	SER
1	А	876	ASN
1	А	890	PRO
1	А	912	LEU
1	А	915	ARG
1	А	946	ASP
1	А	949	ASN
1	А	950	ILE
1	А	970	ARG
1	А	979	ASP
1	А	991	ARG
1	А	1022	ASN
1	А	1055	PRO
1	А	1056	PRO
1	А	1058	ASN
1	A	1078	ASN
1	А	1161	THR
1	A	1165	THR
1	А	1239	ASN
1	А	1242	VAL



Mol	Chain	Res	Type
1	А	1260	TRP
1	А	1287	LYS
1	А	1297	LEU
1	А	1317	ASP
1	А	1318	ARG
1	А	1324	GLN
1	А	1333	GLU
1	А	1369	GLN
1	А	1371	LYS
1	А	1405	THR
1	В	2762	GLU
1	В	2792	ASP
1	В	2793	ILE
1	В	2840	SER
1	В	2890	PRO
1	В	2914	MET
1	В	2915	ARG
1	В	2919	GLU
1	В	2946	ASP
1	В	2947	ASP
1	В	2970	ARG
1	В	2996	ARG
1	В	3020	ASN
1	В	3022	ASN
1	В	3049	GLU
1	В	3053	ASP
1	В	3055	PRO
1	В	3056	PRO
1	В	3070	ASN
1	В	3078	ASN
1	В	3124	ARG
1	В	3140	TRP
1	В	3171	GLN
1	В	3221	ASP
1	В	3238	ARG
1	В	3260	TRP
1	В	3266	ASP
1	В	3272	MET
1	В	3287	LYS
1	B	3324	GLN
1	В	3369	GLN
1	В	3380	PHE



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Mol	Chain	Res	Type
1	В	3405	THR
1	В	3406	ASN
1	В	3411	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	798	HIS
1	А	876	ASN
1	А	949	ASN
1	А	986	ASN
1	А	988	HIS
1	А	1002	ASN
1	А	1004	GLN
1	А	1022	ASN
1	А	1070	ASN
1	А	1078	ASN
1	А	1110	GLN
1	А	1111	GLN
1	А	1123	GLN
1	А	1143	ASN
1	А	1166	GLN
1	А	1239	ASN
1	А	1241	GLN
1	А	1262	GLN
1	А	1264	GLN
1	А	1268	GLN
1	А	1290	HIS
1	А	1324	GLN
1	А	1328	GLN
1	А	1342	GLN
1	А	1369	GLN
1	В	2795	HIS
1	В	2798	HIS
1	В	2846	ASN
1	В	2986	ASN
1	В	3004	GLN
1	В	3020	ASN
1	В	3110	GLN
1	В	3123	GLN
1	В	3166	GLN
1	В	3241	GLN



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Mol	Chain	Res	Type
1	В	3261	GLN
1	В	3262	GLN
1	В	3324	GLN
1	В	3363	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

8 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).

Mal	Tuno	Chain	Dog	Link	B	ond leng	$\operatorname{gths}$	B	Sond ang	gles
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
3	FMN	В	2451	-	33,33,33	4.07	18 (54%)	48,50,50	2.41	17 (35%)
5	NAP	В	2453	-	45,52,52	2.90	10 (22%)	56,80,80	1.77	15 (26%)
2	SO3	А	1500	-	$1,\!3,\!3$	2.51	1 (100%)	0,3,3	-	-
3	FMN	А	1451	-	33,33,33	<mark>3.96</mark>	19 (57%)	48,50,50	2.48	20 (41%)
4	FAD	В	2452	-	$53,\!58,\!58$	<b>5.62</b>	34 (64%)	68,89,89	2.49	24 (35%)
5	NAP	А	1453	-	45,52,52	2.01	9 (20%)	56,80,80	1.55	12 (21%)
4	FAD	А	1452	-	$53,\!58,\!58$	<mark>5.63</mark>	39 (73%)	68,89,89	2.48	26 (38%)
2	SO3	В	2500	-	1,3,3	2.48	1 (100%)	0,3,3	-	-



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	В	2451	-	-	0/18/18/18	0/3/3/3
5	NAP	В	2453	-	-	12/31/67/67	0/5/5/5
3	FMN	А	1451	-	-	0/18/18/18	0/3/3/3
4	FAD	В	2452	-	-	4/30/50/50	0/6/6/6
5	NAP	А	1453	-	-	14/31/67/67	0/5/5/5
4	FAD	А	1452	-	-	4/30/50/50	0/6/6/6

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
4	В	2452	FAD	C4A-N3A	15.31	1.56	1.35
4	В	2452	FAD	C2B-C1B	-14.79	1.31	1.53
4	А	1452	FAD	C2B-C1B	-14.43	1.31	1.53
4	А	1452	FAD	C4A-N3A	14.30	1.55	1.35
4	В	2452	FAD	C2A-N1A	11.66	1.55	1.33
4	А	1452	FAD	C2A-N1A	11.31	1.55	1.33
4	А	1452	FAD	C9A-C5X	11.30	1.60	1.41
4	В	2452	FAD	C1'-C2'	11.25	1.68	1.52
3	В	2451	FMN	C9-C9A	11.23	1.57	1.39
3	А	1451	FMN	C9-C9A	11.15	1.57	1.39
5	В	2453	NAP	C2N-N1N	11.11	1.48	1.35
4	В	2452	FAD	C2A-N3A	11.07	1.50	1.32
4	А	1452	FAD	C2A-N3A	10.82	1.49	1.32
4	В	2452	FAD	C9A-C5X	10.42	1.58	1.41
5	В	2453	NAP	C2D-C1D	-10.32	1.38	1.53
4	А	1452	FAD	C1'-C2'	10.17	1.67	1.52
4	В	2452	FAD	C8A-N7A	-9.05	1.18	1.34
4	А	1452	FAD	C8A-N7A	-8.81	1.19	1.34
4	А	1452	FAD	C8-C7	8.00	1.60	1.40
3	В	2451	FMN	C9A-C5A	7.57	1.53	1.41
4	В	2452	FAD	C4'-C3'	-7.45	1.39	1.53
4	А	1452	FAD	O4'-C4'	7.41	1.59	1.43
5	А	1453	NAP	C2N-N1N	7.33	1.43	1.35
3	А	1451	FMN	C6-C7	7.24	1.50	1.39
4	В	2452	FAD	C8-C7	7.15	1.58	1.40
3	В	2451	FMN	C4-N3	6.90	1.51	1.38
3	В	2451	FMN	C6-C7	6.65	1.49	1.39
4	А	1452	FAD	C4'-C3'	-6.65	1.40	1.53



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
3	А	1451	FMN	C9A-C5A	6.56	1.52	1.41
4	В	2452	FAD	O4'-C4'	6.53	1.57	1.43
4	В	2452	FAD	C10-N10	6.33	1.51	1.37
4	В	2452	FAD	C9-C9A	6.32	1.49	1.39
4	А	1452	FAD	C3B-C4B	-6.31	1.36	1.53
4	А	1452	FAD	C9-C9A	6.29	1.49	1.39
4	А	1452	FAD	P-O2P	-6.16	1.26	1.55
3	В	2451	FMN	C4A-C10	6.00	1.61	1.44
3	В	2451	FMN	C2'-C3'	-5.92	1.42	1.53
3	А	1451	FMN	C2'-C3'	-5.90	1.42	1.53
4	А	1452	FAD	C4X-N5	5.89	1.42	1.30
4	В	2452	FAD	P-O2P	-5.87	1.27	1.55
4	А	1452	FAD	PA-O2A	-5.86	1.27	1.55
5	В	2453	NAP	O4D-C1D	5.84	1.49	1.41
4	А	1452	FAD	C2'-C3'	5.81	1.64	1.53
4	В	2452	FAD	C3B-C4B	-5.76	1.38	1.53
3	А	1451	FMN	C4-N3	5.75	1.49	1.38
4	В	2452	FAD	PA-O2A	-5.71	1.28	1.55
4	А	1452	FAD	O4-C4	-5.46	1.13	1.23
3	А	1451	FMN	C5A-N5	5.28	1.49	1.39
4	В	2452	FAD	O2'-C2'	-5.26	1.32	1.43
3	А	1451	FMN	C4A-C10	5.08	1.59	1.44
4	В	2452	FAD	C4X-N5	5.08	1.40	1.30
5	А	1453	NAP	P2B-O2B	5.01	1.68	1.59
4	А	1452	FAD	C8M-C8	-4.98	1.41	1.51
3	В	2451	FMN	C5A-N5	4.98	1.49	1.39
5	A	1453	NAP	C2D-C1D	-4.96	1.46	1.53
3	A	1451	FMN	C8-C7	4.85	1.53	1.40
4	A	1452	FAD	O2'-C2'	-4.83	1.33	1.43
3	В	2451	FMN	C8-C7	4.82	1.52	1.40
4	A	1452	FAD	C10-N10	4.74	1.47	1.37
4	B	2452	FAD	04-C4	-4.68	1.14	1.23
4	A	1452	FAD	05'-C5'	-4.62	1.27	1.44
4	B	2452	FAD	P-OIP	-4.51	1.34	1.50
3	В	2451	FMN	C9A-N10	4.48	1.49	1.41
	A	1451	FMN	O3'-C3'	4.46	1.53	1.43
	В	2451	FMN	C2-N3	4.45	1.49	1.39
4	В	2452	FAD	O4B-CIB	4.43	1.47	1.41
4	В	2452	FAD	UIU-NI	4.37	1.42	1.33
5	В	2453	NAP DMN	P2B-02B	4.35	1.07	1.59
	B	2451	FMN	C10-N10	4.31	1.46	1.37
4	В	2452	FAD	C2'-C3'	4.26	1.61	1.53



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	В	2453	NAP	C6N-N1N	4.22	1.45	1.35
4	В	2452	FAD	C8M-C8	-4.21	1.42	1.51
4	А	1452	FAD	C5B-C4B	4.16	1.64	1.51
4	А	1452	FAD	C10-N1	4.15	1.41	1.33
4	А	1452	FAD	P-O1P	-4.15	1.36	1.50
3	А	1451	FMN	C10-N10	4.14	1.46	1.37
3	В	2451	FMN	O3'-C3'	4.11	1.52	1.43
3	А	1451	FMN	C6-C5A	4.10	1.46	1.40
4	А	1452	FAD	O2-C2	-4.00	1.16	1.24
4	А	1452	FAD	C1'-N10	3.97	1.58	1.48
3	В	2451	FMN	C6-C5A	3.94	1.46	1.40
4	А	1452	FAD	O3B-C3B	-3.93	1.33	1.43
4	В	2452	FAD	O3'-C3'	3.90	1.52	1.43
3	А	1451	FMN	C2-N3	3.81	1.47	1.39
4	В	2452	FAD	O5'-C5'	-3.78	1.30	1.44
5	А	1453	NAP	C6N-N1N	3.72	1.44	1.35
4	В	2452	FAD	O3B-C3B	-3.72	1.34	1.43
3	В	2451	FMN	O2'-C2'	-3.70	1.35	1.43
4	В	2452	FAD	C6A-C5A	3.70	1.57	1.43
3	А	1451	FMN	O2'-C2'	-3.69	1.35	1.43
4	В	2452	FAD	PA-O1A	-3.68	1.37	1.50
3	А	1451	FMN	C5'-C4'	3.68	1.57	1.51
4	А	1452	FAD	C6A-C5A	3.61	1.56	1.43
4	А	1452	FAD	O4B-C1B	3.58	1.46	1.41
3	А	1451	FMN	C9A-N10	3.51	1.47	1.41
3	В	2451	FMN	C5'-C4'	3.44	1.56	1.51
5	В	2453	NAP	C4N-C3N	3.43	1.45	1.39
4	В	2452	FAD	C1'-N10	3.43	1.56	1.48
5	А	1453	NAP	O4B-C1B	3.31	1.45	1.41
5	А	1453	NAP	O4D-C1D	3.31	1.45	1.41
4	А	1452	FAD	PA-O1A	-3.29	1.39	1.50
4	В	2452	FAD	C5B-C4B	3.25	1.61	1.51
5	В	2453	NAP	O4B-C1B	3.07	1.45	1.41
4	А	1452	FAD	C6-C5X	-3.01	1.35	1.40
4	А	1452	FAD	C5A-N7A	-2.98	1.28	1.39
4	В	2452	FAD	C6A-N6A	2.93	1.44	1.34
3	А	1451	FMN	C4A-C4	-2.89	1.33	1.44
4	В	2452	FAD	C5A-N7A	-2.78	1.29	1.39
5	В	2453	NAP	C2N-C3N	-2.73	1.34	1.39
4	В	2452	FAD	C9-C8	-2.70	1.35	1.39
3	A	1451	FMN	P-O1P	-2.64	1.42	1.50
4	А	1452	FAD	C4-N3	2.60	1.43	1.38



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	А	1453	NAP	C3N-C7N	2.55	1.54	1.50
5	В	2453	NAP	O3D-C3D	2.55	1.49	1.43
2	А	1500	SO3	O1-S	2.51	1.55	1.44
4	А	1452	FAD	C6A-N6A	2.51	1.43	1.34
5	А	1453	NAP	C2D-C3D	-2.50	1.46	1.53
2	В	2500	SO3	O1-S	2.48	1.54	1.44
3	В	2451	FMN	C4A-C4	-2.44	1.35	1.44
4	А	1452	FAD	O3'-C3'	2.40	1.48	1.43
3	В	2451	FMN	P-O3P	-2.39	1.45	1.54
5	А	1453	NAP	C4N-C3N	2.38	1.43	1.39
4	А	1452	FAD	C9-C8	-2.31	1.36	1.39
3	В	2451	FMN	P-O1P	-2.28	1.43	1.50
4	А	1452	FAD	C6-C7	-2.24	1.36	1.39
3	А	1451	FMN	C7M-C7	-2.20	1.46	1.51
3	А	1451	FMN	P-O3P	-2.11	1.46	1.54
4	В	2452	FAD	C4-N3	2.11	1.42	1.38
5	В	2453	NAP	C3D-C4D	-2.09	1.47	1.53
4	А	1452	FAD	$C\overline{2B}-C\overline{3B}$	-2.05	1.47	1.53
4	A	1452	FAD	C4X-C10	-2.00	1.38	1.44

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
4	А	1452	FAD	C1B-N9A-C4A	-7.13	114.12	126.64
4	В	2452	FAD	C1B-N9A-C4A	-6.92	114.48	126.64
4	А	1452	FAD	C5X-C9A-N10	-6.45	111.29	117.95
4	В	2452	FAD	C5X-C9A-N10	-6.31	111.44	117.95
3	А	1451	FMN	C7M-C7-C6	-6.26	107.92	119.49
3	В	2451	FMN	C7M-C7-C6	-6.23	107.98	119.49
4	В	2452	FAD	O5'-P-O1P	-5.70	86.79	109.07
4	А	1452	FAD	O5'-P-O1P	-5.68	86.89	109.07
4	В	2452	FAD	N3A-C2A-N1A	-5.43	120.18	128.68
4	В	2452	FAD	C3B-C2B-C1B	5.34	109.02	100.98
3	А	1451	FMN	C9A-C5A-N5	-5.22	116.76	122.43
4	А	1452	FAD	N3A-C2A-N1A	-5.06	120.77	128.68
5	В	2453	NAP	N3A-C2A-N1A	-5.01	120.85	128.68
4	А	1452	FAD	C3B-C2B-C1B	4.97	108.46	100.98
3	В	2451	FMN	C9A-C5A-N5	-4.93	117.08	122.43
3	А	1451	FMN	O2-C2-N1	4.90	129.95	121.83
4	А	1452	FAD	C4A-C5A-N7A	4.84	114.45	109.40
4	В	2452	FAD	C4A-C5A-N7A	4.83	114.43	109.40
3	В	2451	FMN	C10-N1-C2	4.82	126.54	116.90



11	TT	Т
Т	ΤL	L.

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	А	1453	NAP	N3A-C2A-N1A	-4.73	121.29	128.68
4	А	1452	FAD	C9-C9A-N10	4.69	128.17	121.84
3	В	2451	FMN	C7M-C7-C8	4.66	130.29	120.74
3	А	1451	FMN	C10-N1-C2	4.65	126.21	116.90
4	В	2452	FAD	P-O3P-PA	-4.60	117.03	132.83
3	В	2451	FMN	C5A-C9A-N10	4.59	122.69	117.95
3	А	1451	FMN	C7M-C7-C8	4.59	130.15	120.74
3	А	1451	FMN	C5A-C9A-N10	4.50	122.60	117.95
3	В	2451	FMN	O2-C2-N1	4.40	129.12	121.83
4	А	1452	FAD	P-O3P-PA	-4.33	117.95	132.83
4	В	2452	FAD	O5B-PA-O1A	-4.32	92.19	109.07
4	В	2452	FAD	C9-C9A-N10	4.31	127.66	121.84
3	А	1451	FMN	O4-C4-N3	-4.04	112.37	120.12
4	А	1452	FAD	C2A-N1A-C6A	3.86	125.36	118.75
5	А	1453	NAP	O4D-C1D-C2D	3.86	112.56	106.93
3	В	2451	FMN	O4-C4-N3	-3.78	112.88	120.12
4	А	1452	FAD	O5B-PA-O1A	-3.69	94.63	109.07
4	В	2452	FAD	C2A-N1A-C6A	3.67	125.04	118.75
4	А	1452	FAD	O4B-C4B-C3B	-3.50	98.18	105.11
5	В	2453	NAP	C5N-C4N-C3N	3.44	124.42	120.34
3	В	2451	FMN	O3P-P-O2P	3.40	120.64	107.64
5	В	2453	NAP	C4A-C5A-N7A	3.34	112.88	109.40
3	A	1451	FMN	O3P-P-O2P	3.29	120.22	107.64
3	В	2451	FMN	C5A-N5-C4A	3.26	123.50	118.07
3	А	1451	FMN	C5A-N5-C4A	3.24	123.47	118.07
4	В	2452	FAD	O4B-C4B-C5B	-3.17	98.95	109.37
5	В	2453	NAP	N6A-C6A-N1A	3.16	125.13	118.57
4	А	1452	FAD	C9A-N10-C10	3.08	125.56	120.77
4	В	2452	FAD	O2'-C2'-C1'	3.04	117.15	109.80
4	В	2452	FAD	O3'-C3'-C2'	-3.00	101.57	108.81
4	В	2452	FAD	C9A-N10-C10	2.99	125.43	120.77
5	А	1453	NAP	C4A-C5A-N7A	2.98	112.50	109.40
4	А	1452	FAD	C10-N1-C2	2.94	122.78	116.90
4	А	1452	FAD	O4B-C4B-C5B	-2.93	99.73	109.37
5	А	1453	NAP	PN-O3-PA	2.89	142.75	132.83
4	В	2452	FAD	C1'-C2'-C3'	2.89	117.87	109.79
4	А	1452	FAD	O3'-C3'-C2'	-2.85	101.92	108.81
5	A	1453	NAP	N6A-C6A-N1A	2.84	124.47	118.57
3	А	1451	FMN	O5'-C5'-C4'	-2.83	101.80	109.36
5	В	2453	NAP	O7N-C7N-C3N	-2.82	116.25	119.63
3	А	1451	FMN	C6-C5A-N5	2.82	123.43	118.51
5	В	2453	NAP	O3D-C3D-C4D	2.81	119.19	111.05
	1	1	1	1	1	1	1



11	TT	Т
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	Ideal(°)
4	А	1452	FAD	C7M-C7-C6	-2.80	114.32	119.49
5	В	2453	NAP	C3N-C2N-N1N	-2.79	117.70	120.43
3	В	2451	FMN	C4A-C10-N1	-2.79	118.27	124.73
3	В	2451	FMN	C9A-N10-C10	-2.77	116.45	120.77
5	В	2453	NAP	C5D-C4D-C3D	-2.77	104.80	115.18
4	В	2452	FAD	O4B-C4B-C3B	-2.75	99.67	105.11
4	В	2452	FAD	C2B-C3B-C4B	2.75	107.98	102.64
4	А	1452	FAD	C1'-C2'-C3'	2.74	117.44	109.79
3	А	1451	FMN	C4A-C10-N1	-2.64	118.60	124.73
5	А	1453	NAP	O4B-C4B-C5B	-2.64	100.69	109.37
4	В	2452	FAD	C8M-C8-C9	-2.62	114.64	119.49
4	В	2452	FAD	C10-N1-C2	2.56	122.01	116.90
4	А	1452	FAD	C4X-C4-N3	2.52	119.60	113.19
5	В	2453	NAP	O5B-C5B-C4B	-2.50	100.38	108.99
3	В	2451	FMN	C6-C5A-N5	2.50	122.87	118.51
4	А	1452	FAD	C8M-C8-C9	-2.49	114.89	119.49
5	В	2453	NAP	PN-O3-PA	2.48	141.33	132.83
3	В	2451	FMN	O5'-C5'-C4'	-2.47	102.76	109.36
4	В	2452	FAD	C7M-C7-C6	-2.47	114.93	119.49
5	В	2453	NAP	O2N-PN-O5D	2.42	118.99	107.75
3	А	1451	FMN	C9A-N10-C10	-2.42	117.00	120.77
5	А	1453	NAP	C3N-C2N-N1N	-2.41	118.08	120.43
5	В	2453	NAP	O3X-P2B-O2X	2.40	116.82	107.64
5	В	2453	NAP	O3D-C3D-C2D	2.39	119.55	111.82
5	А	1453	NAP	O2N-PN-O5D	2.38	118.79	107.75
4	А	1452	FAD	O2'-C2'-C1'	2.38	115.55	109.80
5	А	1453	NAP	O5B-C5B-C4B	-2.34	100.92	108.99
5	В	2453	NAP	C2D-C3D-C4D	-2.34	98.09	102.64
3	В	2451	FMN	C1'-N10-C9A	2.34	124.41	120.51
5	А	1453	NAP	C5N-C4N-C3N	2.33	123.11	120.34
3	А	1451	FMN	N3-C2-N1	-2.29	114.89	119.38
5	А	1453	NAP	C5D-C4D-C3D	-2.29	106.60	115.18
3	А	1451	FMN	C5'-C4'-C3'	2.28	116.61	112.20
4	А	1452	FAD	C2B-C3B-C4B	2.27	107.05	102.64
4	В	2452	FAD	C4X-C4-N3	2.26	118.92	113.19
4	A	1452	FAD	C4-N3-C2	-2.25	121.48	125.64
3	А	1451	FMN	C4'-C3'-C2'	2.25	118.04	113.36
4	A	1452	FAD	C7M-C7-C8	2.24	125.32	120.74
4	А	1452	FAD	O2P-P-O1P	2.22	123.22	112.24
3	A	1451	FMN	C4A-C10-N10	2.21	119.72	116.48
4	А	1452	FAD	C4X-C10-N1	-2.20	119.64	124.73
3	В	2451	FMN	C4A-C10-N10	2.19	119.68	116.48



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	В	2452	FAD	O2P-P-O5'	2.14	117.67	107.75
3	А	1451	FMN	C1'-N10-C9A	2.12	124.04	120.51
5	В	2453	NAP	O5D-C5D-C4D	2.12	116.27	108.99
5	А	1453	NAP	O7N-C7N-C3N	-2.10	117.12	119.63
3	А	1451	FMN	C10-C4A-N5	-2.10	120.41	124.86
3	В	2451	FMN	N3-C2-N1	-2.06	115.33	119.38
4	В	2452	FAD	C4X-C10-N1	-2.06	119.95	124.73
3	А	1451	FMN	O3'-C3'-C4'	-2.06	103.84	108.81
4	А	1452	FAD	O2P-P-O5'	2.02	117.13	107.75
3	В	2451	FMN	C10-C4A-N5	-2.01	120.59	124.86
4	В	2452	FAD	C7M-C7-C8	2.00	124.84	120.74

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	1453	NAP	C5B-O5B-PA-O3
5	А	1453	NAP	C5D-O5D-PN-O1N
5	А	1453	NAP	C5D-O5D-PN-O2N
5	А	1453	NAP	O4D-C1D-N1N-C6N
5	В	2453	NAP	C5B-O5B-PA-O1A
5	В	2453	NAP	C5B-O5B-PA-O2A
5	В	2453	NAP	C5B-O5B-PA-O3
5	В	2453	NAP	C5D-O5D-PN-O3
5	В	2453	NAP	O4D-C4D-C5D-O5D
5	А	1453	NAP	C3B-C4B-C5B-O5B
5	А	1453	NAP	O4D-C4D-C5D-O5D
5	В	2453	NAP	C3B-C4B-C5B-O5B
5	А	1453	NAP	O4B-C4B-C5B-O5B
5	А	1453	NAP	C3D-C4D-C5D-O5D
5	В	2453	NAP	O4B-C4B-C5B-O5B
5	В	2453	NAP	C3D-C4D-C5D-O5D
4	А	1452	FAD	O2'-C2'-C3'-O3'
4	В	2452	FAD	O2'-C2'-C3'-O3'
4	А	1452	FAD	O2'-C2'-C3'-C4'
4	В	2452	FAD	O4B-C4B-C5B-O5B
4	В	2452	FAD	O2'-C2'-C3'-C4'
5	А	1453	NAP	PA-O3-PN-O5D
5	В	2453	NAP	PA-O3-PN-O5D
4	В	2452	FAD	C3B-C4B-C5B-O5B
5	A	1453	NAP	C5B-O5B-PA-O1A
5	А	1453	NAP	C5B-O5B-PA-O2A



Mol	Chain	Res	Type	Atoms
5	В	2453	NAP	C5D-O5D-PN-O1N
4	А	1452	FAD	P-O3P-PA-O1A
4	А	1452	FAD	O4B-C4B-C5B-O5B
5	А	1453	NAP	C5D-O5D-PN-O3
5	А	1453	NAP	C2D-C1D-N1N-C2N
5	В	2453	NAP	C2D-C1D-N1N-C2N
5	А	1453	NAP	C4D-C5D-O5D-PN
5	В	2453	NAP	C4D-C5D-O5D-PN

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There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	В	2453	NAP	13	0
5	А	1453	NAP	9	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 sufficient 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	630/688~(91%)	0.61	52 (8%) 11 15	28, 52, 88, 99	0
1	В	616/688~(89%)	0.84	84 (13%) 3 4	24, 61, 93, 100	0
All	All	1246/1376~(90%)	0.73	136 (10%) 5 8	24, 56, 92, 100	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	830	HIS	9.8
1	В	2902	LEU	8.7
1	В	3316	PRO	8.0
1	В	2845	PHE	7.5
1	А	950	ILE	7.2
1	В	3413	ILE	7.1
1	В	2843	VAL	6.9
1	В	2948	VAL	6.0
1	А	948	VAL	5.9
1	В	3371	LYS	5.7
1	В	2967	ASN	5.6
1	А	1073	LEU	5.6
1	В	3073	LEU	5.4
1	В	3411	GLU	5.2
1	А	1413	ILE	5.0
1	В	2794	VAL	4.8
1	В	2947	ASP	4.7
1	В	2752	ARG	4.7
1	В	2906	LEU	4.7
1	В	3402	TYR	4.6
1	А	838	ARG	4.5
1	А	1057	ALA	4.4
1	В	2779	HIS	4.3
1	В	2949	ASN	4.3



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Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	В	2826	MET	4.3
1	А	837	GLU	4.2
1	А	839	LYS	4.2
1	В	2793	ILE	4.2
1	В	3373	SER	4.2
1	А	1157	GLN	4.1
1	В	3408	LEU	4.1
1	А	843	VAL	4.0
1	В	2825	LEU	4.0
1	А	946	ASP	3.9
1	А	966	ARG	3.9
1	В	2961	ASP	3.9
1	А	959	SER	3.8
1	А	973	TYR	3.8
1	В	3366	MET	3.8
1	В	3412	SER	3.7
1	В	3318	ARG	3.7
1	А	1374	GLU	3.7
1	А	1071	THR	3.7
1	В	2822	GLY	3.6
1	В	3317	ASP	3.6
1	В	3407	ARG	3.6
1	В	2944	VAL	3.5
1	В	3372	LEU	3.5
1	В	2791	TYR	3.5
1	А	750	ALA	3.4
1	А	1116	ALA	3.4
1	В	2909	GLU	3.4
1	А	1317	ASP	3.4
1	В	3410	SER	3.4
1	В	2784	LYS	3.4
1	А	849	SER	3.3
1	В	2780	ALA	3.3
1	В	2894	ALA	3.3
1	А	1383	ARG	3.3
1	А	836	GLU	3.2
1	В	2877	VAL	3.1
1	В	3076	ILE	3.1
1	А	1079	TRP	3.0
1	В	2846	ASN	3.0
1	В	2898	ALA	3.0
1	А	842	LYS	2.9



Mol	Chain	Res	Type	RSRZ
1	А	1117	THR	2.9
1	В	2842	LYS	2.9
1	В	2905	GLU	2.9
1	А	1375	GLU	2.9
1	В	2796	LEU	2.9
1	А	1121	GLU	2.8
1	В	2828	MET	2.8
1	В	2844	ARG	2.7
1	В	2920	LEU	2.7
1	А	1318	ARG	2.7
1	А	945	GLY	2.7
1	А	1254	ALA	2.6
1	В	3072	ALA	2.6
1	В	2819	GLU	2.6
1	В	2827	GLU	2.6
1	А	1076	ILE	2.6
1	В	2915	ARG	2.6
1	А	1119	GLU	2.6
1	А	1132	LEU	2.5
1	В	3120	LYS	2.5
1	А	1364	ARG	2.5
1	В	3253	ILE	2.5
1	А	847	SER	2.5
1	В	2765	LYS	2.5
1	В	3376	ASP	2.5
1	В	3140	TRP	2.5
1	В	2766	SER	2.5
1	В	2841	TYR	2.5
1	В	3119	GLU	2.5
1	В	3383	ARG	2.4
1	В	2753	VAL	2.4
1	А	846	ASN	2.4
1	А	1054	ALA	2.4
1	A	751	LYS	2.4
1	А	1120	LYS	2.4
1	B	3127	VAL	2.3
1	A	1058	ASN	2.3
1	В	3378	GLY	2.3
1	A	1403	GLU	2.3
1	В	2950	ILE	2.3
1	B	2903	LEU	2.2
1	В	3201	ASP	2.2



Mol	Chain	Res	Type	RSRZ
1	В	3285	GLN	2.2
1	А	976	GLU	2.2
1	В	3287	LYS	2.2
1	А	964	TRP	2.2
1	В	3068	GLU	2.2
1	В	3246	LEU	2.2
1	А	1130	LYS	2.2
1	А	1246	LEU	2.2
1	А	963	SER	2.2
1	В	3130	LYS	2.1
1	В	3116	ALA	2.1
1	В	2976	GLU	2.1
1	А	1280	VAL	2.1
1	В	3066	LEU	2.1
1	В	3379	VAL	2.1
1	А	1175	TYR	2.1
1	В	2789	GLU	2.1
1	В	3349	CYS	2.1
1	А	960	ASN	2.1
1	В	2817	ASN	2.1
1	В	2946	ASP	2.1
1	А	1072	ALA	2.1
1	В	3176	SER	2.0
1	В	3377	ALA	2.0
1	А	1407	ARG	2.0
1	В	3053	ASP	2.0
1	В	3058	ASN	2.0
1	В	3174	TYR	2.0

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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,





Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	$Q{<}0.9$
2	SO3	А	1500	4/4	0.83	0.22	$67,\!68,\!68,\!68$	4
5	NAP	В	2453	48/48	0.87	0.18	40,47,59,61	0
5	NAP	А	1453	48/48	0.92	0.17	$27,\!44,\!54,\!56$	0
2	SO3	В	2500	4/4	0.92	0.13	79,80,81,82	0
4	FAD	В	2452	53/53	0.96	0.16	17,29,59,59	0
3	FMN	А	1451	31/31	0.96	0.17	32,35,38,41	0
3	FMN	В	2451	31/31	0.96	0.18	45,49,53,54	0
4	FAD	А	1452	53/53	0.97	0.17	17,30,51,53	0

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.

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.

