



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:15 PM GMT

PDB ID : 1TLL
Title : CRYSTAL STRUCTURE OF RAT NEURONAL NITRIC-OXIDE SYNTHASE REDUCTASE MODULE AT 2.3 Å RESOLUTION.
Authors : Garcin, E.D.; Bruns, C.M.; Lloyd, S.J.; Hosfield, D.J.; Tiso, M.; Gachhui, R.; Stuehr, D.J.; Tainer, J.A.; Getzoff, E.D.
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

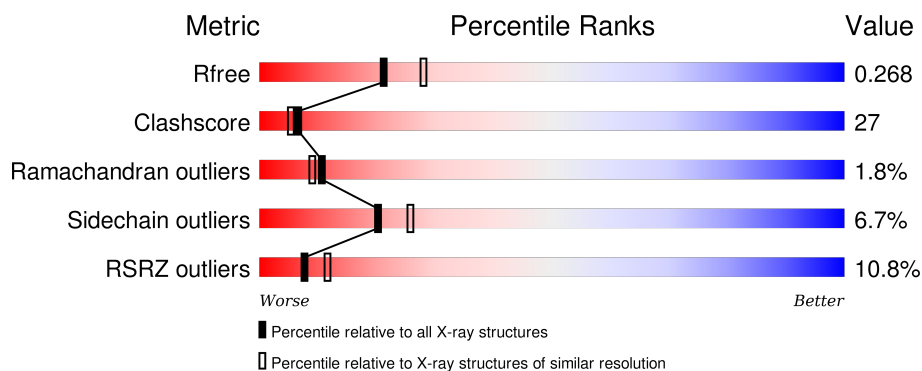
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	688	
1	B	688	

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.

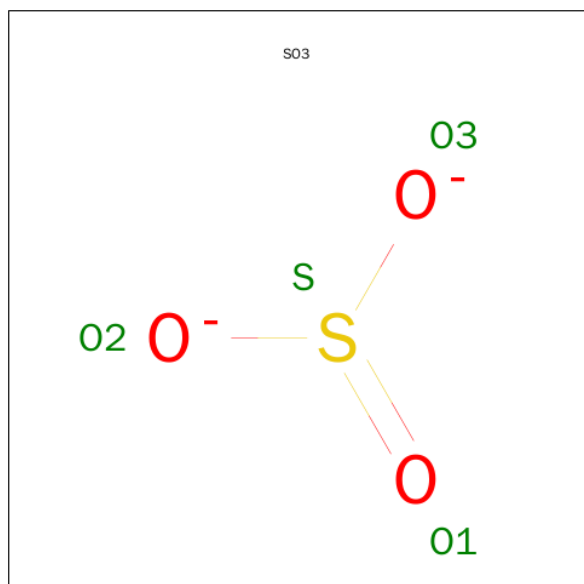
- Molecule 1 is a protein called Nitric-oxide synthase, brain.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1008	SER	PHE	SEE REMARK 999	UNP P29476
B	3008	SER	PHE	SEE REMARK 999	UNP P29476

- Molecule 2 is SULFITE ION (three-letter code: SO3) (formula: O₃S).



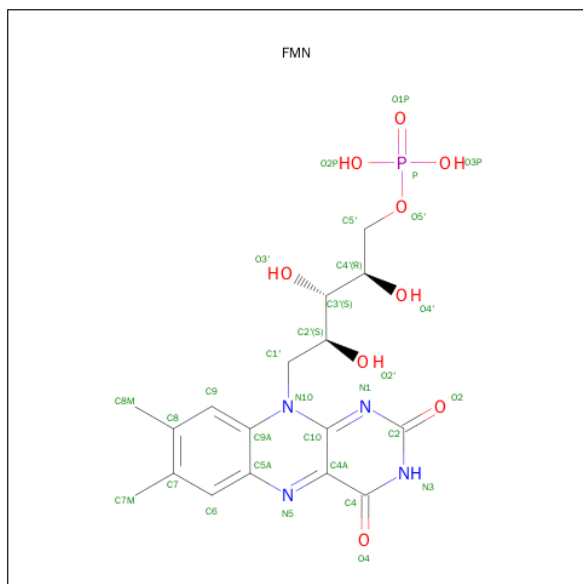
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O S	0	0
			4	3 1		

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

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



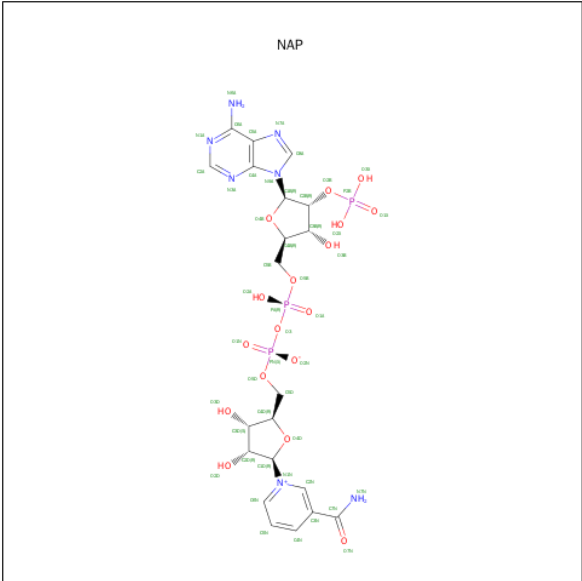
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



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

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

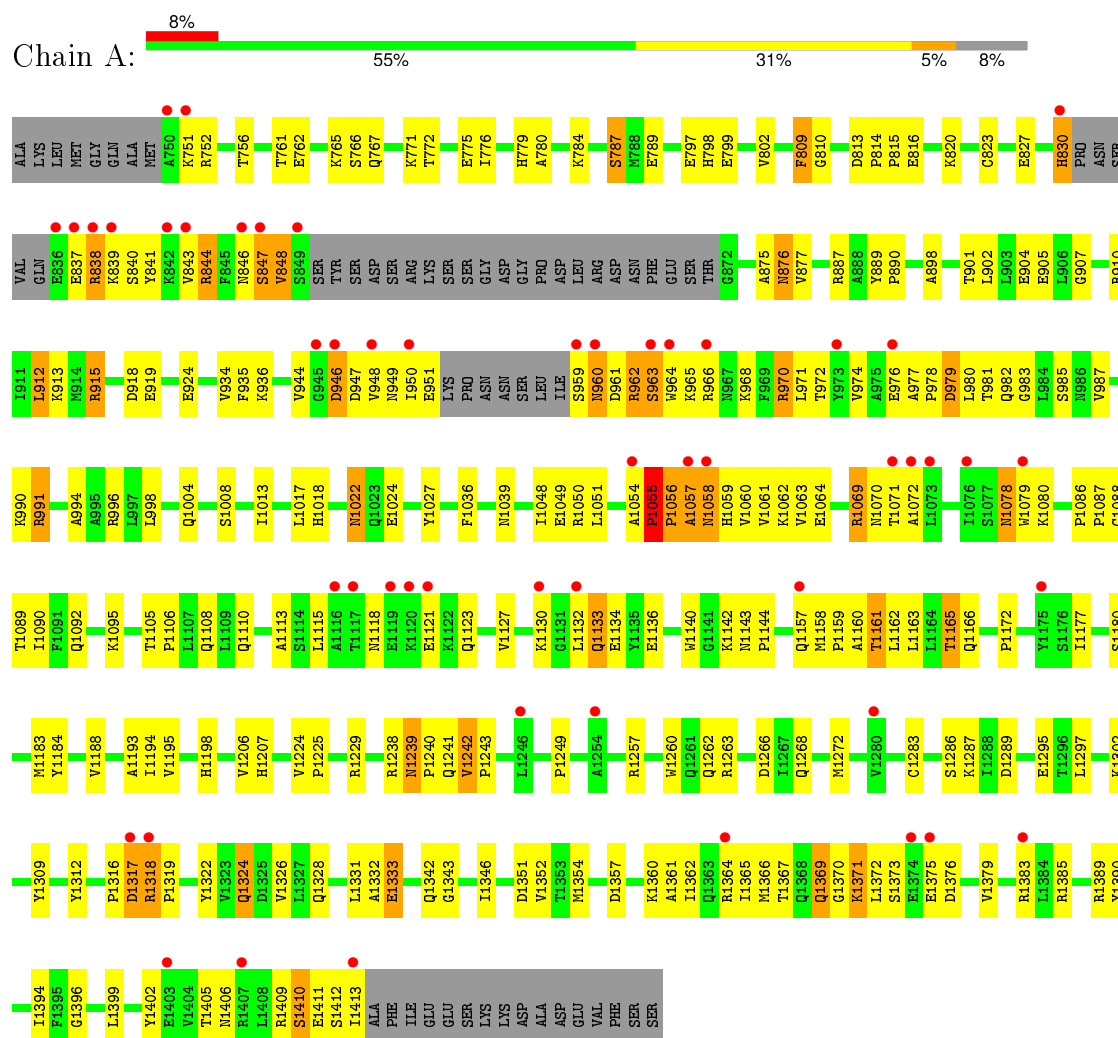
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	127	Total	O	0	0
			127	127		
6	B	96	Total	O	0	0
			96	96		

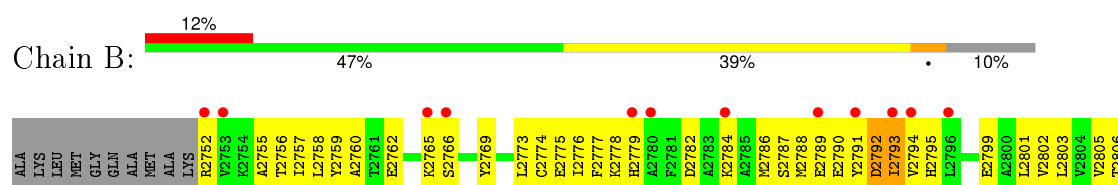
3 Residue-property plots

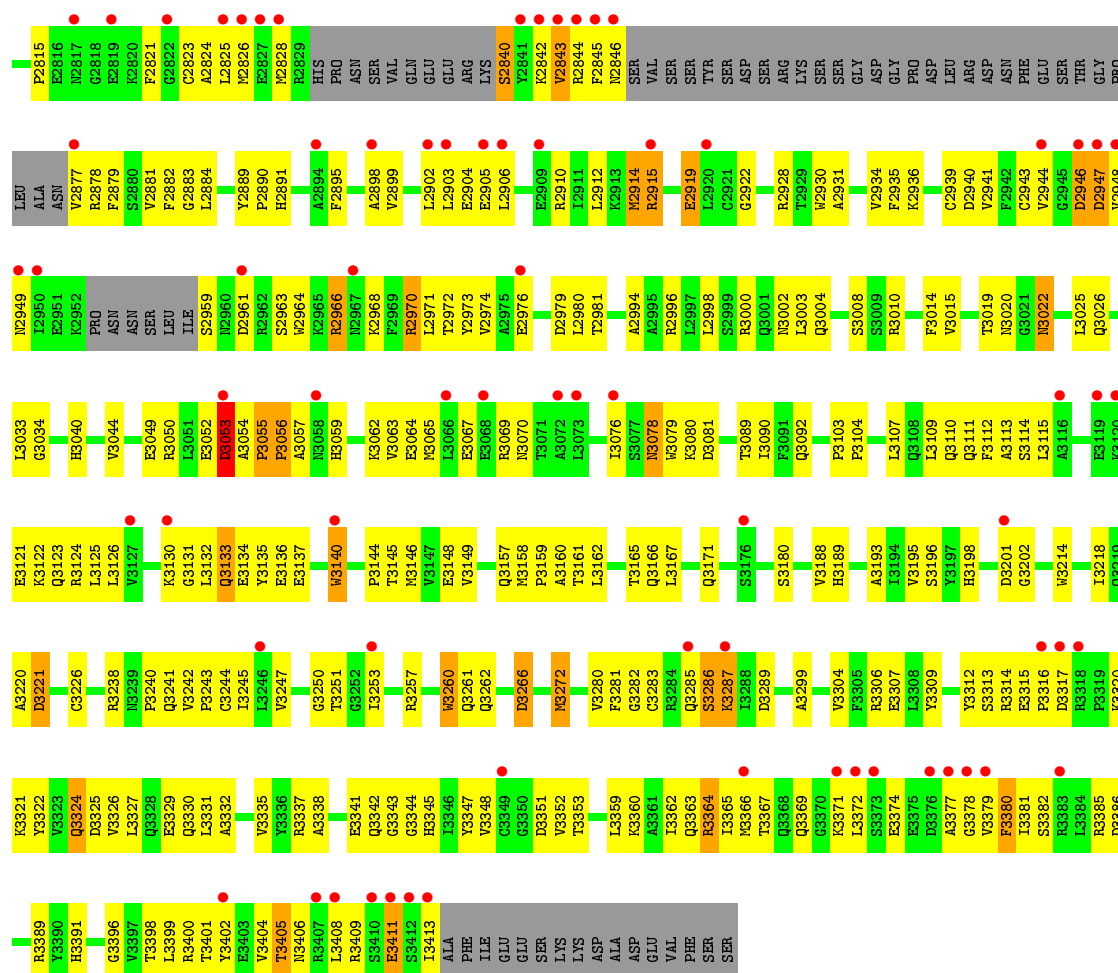
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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



- Molecule 1: Nitric-oxide synthase, brain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.76Å 69.17Å 82.63Å 76.80° 72.07° 67.14°	Depositor
Resolution (Å)	35.21 – 2.30 35.21 – 2.17	Depositor EDS
% Data completeness (in resolution range)	97.8 (35.21-2.30) 92.2 (35.21-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.272 0.239 , 0.268	Depositor DCC
R_{free} test set	1909 reflections (3.59%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 64025 reflections	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, NAP, SO3, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	2/5122 (0.0%)	0.71	2/6932 (0.0%)
1	B	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	Z	Observed(Å)	Ideal(Å)
1	A	1133	GLN	CA-CB	-5.70	1.41	1.53
1	A	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(°)	Ideal(°)
1	B	3364	ARG	NE-CZ-NH1	19.58	130.09	120.30
1	B	3364	ARG	NE-CZ-NH2	-16.65	111.97	120.30
1	B	2944	VAL	N-CA-C	-6.22	94.21	111.00
1	B	2966	ARG	N-CA-C	5.69	126.37	111.00
1	B	3364	ARG	CD-NE-CZ	5.38	131.14	123.60
1	A	1133	GLN	CB-CG-CD	-5.15	98.22	111.60
1	B	2943	CYS	N-CA-C	5.06	124.67	111.00
1	A	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 ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5010	0	4925	260	1
1	B	4903	0	4814	287	1
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	31	0	18	0	0
3	B	31	0	18	0	0
4	A	53	0	28	0	0
4	B	53	0	28	0	0
5	A	48	0	24	9	0
5	B	48	0	24	13	0
6	A	127	0	0	2	0
6	B	96	0	0	6	0
All	All	10408	0	9879	545	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 27.

All (545) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1453:NAP:O3D	5:A:1453:NAP:O2A	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:HH11	1:A:991:ARG:HG3	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:HD22	1:A:1078:ASN:N	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:NE2	1:B:3324:GLN:H	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:NE2	1:A:1324:GLN:H	1.79	0.81
1:B:3324:GLN:HE21	1:B:3324:GLN:N	1.76	0.81
1:B:3360:LYS:O	1:B:3364:ARG:HD2	1.78	0.80
1:A:1062:LYS:HE3	1:A:1087:PRO:HG3	1.62	0.80
1:A:1328:GLN:NE2	1:A:1361:ALA:HA	1.96	0.80
1:A:1324:GLN:N	1:A:1324:GLN:HE21	1.80	0.79
1:B:2842:LYS:HD3	1:B:2846:ASN:HD22	1.47	0.79
1:A:1328:GLN:NE2	1:A:1364:ARG:HD2	1.98	0.79
1:A:1048:ILE:HG21	1:A:1057:ALA:HB2	1.64	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:B:3053:ASP:HB2	1:B:3160:ALA:N	1.96	0.75
1:A:1158:MET:CE	1:A:1162:LEU:HB3	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3162:LEU:HD12	1:B:3166:GLN:CG	2.17	0.74
1:A:1078:ASN:ND2	1:A:1078:ASN:N	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:B:2966:ARG:O	1:B:2966:ARG:HG3	1.90	0.72
1:A:1243:PRO:HG3	1:A:1342:GLN:HE21	1.54	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:B:3111:GLN:O	1:B:3115:LEU:HD12	1.92	0.69
1:A:946:ASP:O	1:A:946:ASP:OD1	2.09	0.69
1:B:3053:ASP:CB	1:B:3160:ALA:H	1.97	0.69
1:A:1062:LYS:HE3	1:A:1087:PRO:CG	2.21	0.69
1:A:799:GLU:HG2	1:A:802:VAL:HG22	1.74	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:B:2878:ARG:HH12	1:B:2941:VAL:HG13	1.58	0.69
1:A:1158:MET:HE3	1:A:1162:LEU:HB3	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3240:PRO:HG2	1:B:3241:GLN:HE21	1.57	0.68
1:B:3322:TYR:HB3	1:B:3324:GLN:NE2	2.07	0.68
1:A:1022:ASN:ND2	1:A:1024:GLU:HG2	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:991:ARG:NH1	1:A:991:ARG:HG3	1.92	0.67
1:A:765:LYS:NZ	1:A:919:GLU:HG3	2.10	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:1324:GLN:HE22	5:A:1453:NAP:C2A	2.07	0.66
1:A:1078:ASN:H	1:A:1078:ASN:HD22	1.44	0.66
1:A:848:VAL:O	1:A:848:VAL:HG12	1.94	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:B:3283:CYS:HB2	1:B:3289:ASP:CB	2.27	0.64
1:A:1058:ASN:O	1:A:1058:ASN:CG	2.36	0.64
1:A:1268:GLN:HE21	1:A:1302:LYS:HD3	1.62	0.64
1:B:3158:MET:HE3	1:B:3159:PRO:HD2	1.79	0.63
1:B:3019:THR:CG2	1:B:3025:LEU:HB2	2.28	0.63
1:B:2946:ASP:N	1:B:2946:ASP:OD2	2.30	0.63
1:A:1328:GLN:HE22	1:A:1364:ARG:HD2	1.61	0.63
1:A:1069:ARG:HG2	1:A:1070:ASN:N	2.12	0.63
1:A:1048:ILE:HD13	1:A:1057:ALA:HB1	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:3286:SER:HB3	1:B:3312:TYR:CZ	2.34	0.62
1:B:2884:LEU:N	1:B:2884:LEU:HD12	2.14	0.62
1:A:1283:CYS:HB2	1:A:1289:ASP:HB3	1.82	0.62
1:B:2971:LEU:CD1	1:B:3055:PRO:HG2	2.29	0.62
1:B:2774:CYS:O	1:B:2778:LYS:HG2	2.00	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:NH1	1:A:991:ARG:CG	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:B:3193:ALA:CB	5:B:2453:NAP:H51N	2.30	0.59
1:A:1162:LEU:HD12	1:A:1166:GLN:HG2	1.84	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:B:3019:THR:O	1:B:3022:ASN:HB2	2.03	0.58
1:B:2842:LYS:HD3	1:B:2846:ASN:ND2	2.16	0.58
1:A:1268:GLN:NE2	1:A:1302:LYS:HD3	2.17	0.58
1:B:3247:VAL:HG23	1:B:3348:VAL:HA	1.85	0.58
1:B:2973:TYR:HE2	1:B:3059:HIS:HD2	1.52	0.58
1:B:3324:GLN:NE2	5:B:2453:NAP:H2A	2.18	0.58
1:A:924:GLU:HG3	1:A:1106:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:1367:THR:HG23	1:A:1372:LEU:O	2.04	0.57
1:A:765:LYS:HZ3	1:A:919:GLU:HG3	1.69	0.57
1:B:2981:THR:HG21	1:B:2994:ALA:HB2	1.86	0.57
1:B:3360:LYS:CB	1:B:3364:ARG:NH1	2.64	0.57
1:B:2793:ILE:HG13	1:B:2793:ILE:O	2.04	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:971:LEU:CD2	1:A:1063:VAL:HG22	2.35	0.57
1:A:767:GLN:O	1:A:771:LYS:HG2	2.05	0.57
1:B:2821:PHE:HE1	1:B:2825:LEU:HD11	1.68	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:2912:LEU:HD21	1:B:2915:ARG:HH12	1.68	0.56
1:A:775:GLU:HG2	1:A:961:ASP:HB2	1.83	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: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: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: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:A:1410:SER:O	1:A:1412:SER:N	2.39	0.56
1:B:2766:SER:OG	1:B:2884:LEU:HD22	2.05	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:3257:ARG:O	1:B:3261:GLN:HG3	2.05	0.56
1:B:2979:ASP:OD1	1:B:2980:LEU:N	2.38	0.56
1:A:981:THR:HG21	1:A:994:ALA:HB2	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:B:2760:ALA:HB1	1:B:2815:PRO:CG	2.37	0.55
1:A:1346:ILE:HD13	1:A:1362:ILE:CD1	2.37	0.55
1:A:1194:ILE:O	5:A:1453:NAP:H5N	2.07	0.55
1:A:1057:ALA:HA	1:A:1090:ILE:HG12	1.89	0.55
1:B:3110:GLN:O	1:B:3113:ALA:HB3	2.07	0.55
1:B:2757:ILE:HG12	1:B:2803:LEU:HB2	1.89	0.55
1:A:1316:PRO:HG2	1:A:1317:ASP:OD1	2.05	0.55
1:A:1056:PRO:C	1:A:1058:ASN:H	2.11	0.54
1:A:1051:LEU:HD21	1:A:1163:LEU:HD12	1.89	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: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:762:GLU:HB2	1:A:809:PHE:CE1	2.43	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:1036:PHE:CE1	1:A:1172:PRO:HB3	2.43	0.54
1:A:756:THR:OG1	1:A:799:GLU:OE2	2.25	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:3351:ASP:OD1	1:B:3353:THR:HB	2.07	0.53
1:B:2843:VAL:HG22	1:B:3382:SER:OG	2.09	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3054:ALA:O	1:B:3056:PRO:HD3	2.09	0.52
1:A:1394:ILE:HG22	1:A:1396:GLY:H	1.73	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:3309:TYR:CD2	1:B:3331:LEU:HD11	2.45	0.52
1:B:2752:ARG:HD2	1:B:2782:ASP:HB2	1.91	0.52
1:B:3019:THR:HG21	1:B:3025:LEU:HB2	1.89	0.52
1:B:2840:SER:O	1:B:2843:VAL:HB	2.09	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:3363:GLN:HA	1:B:3381:ILE:HD11	1.92	0.52
1:B:3245:ILE:HD13	1:B:3335:VAL:HG22	1.91	0.52
1:A:970:ARG:HB3	1:A:1079:TRP:CZ3	2.44	0.52
1:B:3162:LEU:HD12	1:B:3166:GLN:HG3	1.90	0.52
1:A:1286:SER:HA	1:A:1312:TYR:CE2	2.44	0.52
1:B:3242:VAL:CG1	1:B:3344:GLY:HA2	2.38	0.52
1:B:3313:SER:O	1:B:3320:LYS:HE3	2.10	0.51
1:A:1162:LEU:HD12	1:A:1166:GLN:CG	2.40	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: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:1143:ASN:O	1:A:1207:HIS:HE1	1.94	0.51
1:A:1360:LYS:O	1:A:1364:ARG:HG3	2.11	0.51
1:A:775:GLU:CG	1:A:961:ASP:HB2	2.41	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:B:2821:PHE:CE1	1:B:2825:LEU:HD11	2.45	0.51
1:A:1318:ARG:HB2	1:A:1319:PRO:HD2	1.92	0.51
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:1058:ASN:HA	1:A:1089:THR:HB	1.93	0.50
1:A:1195:VAL:HA	5:A:1453:NAP:C5N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1071:THR:CG2	1:A:1072:ALA:N	2.59	0.50
1:A:964:TRP:CH2	1:A:966:ARG:HG3	2.46	0.50
1:B:3015:VAL:O	1:B:3189:HIS:HA	2.12	0.50
1:A:904:GLU:OE2	1:A:910:ARG:NH1	2.42	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:3360:LYS:HE2	1:B:3360:LYS:HA	1.94	0.50
1:B:3076:ILE:HG23	1:B:3076:ILE:O	2.11	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:ND2	1:A:1239:ASN:C	2.64	0.49
1:A:979:ASP:C	1:A:979:ASP:OD1	2.50	0.49
1:A:898:ALA:O	1:A:902:LEU:HG	2.12	0.49
1:B:3145:THR:O	1:B:3149:VAL:HG23	2.12	0.49
1:B:2790:GLU:HG2	1:B:2790:GLU:O	2.12	0.49
1:A:1140:TRP:CD1	1:A:1409:ARG:HD2	2.47	0.49
1:B:3004:GLN:NE2	1:B:3008:SER:OG	2.46	0.49
1:A:1022:ASN:ND2	1:A:1024:GLU:CG	2.73	0.49
1:A:971:LEU:HD23	1:A:1063:VAL:HG22	1.95	0.49
1:A:910:ARG:HD3	1:A:913:LYS:HA	1.95	0.49
1:B:2959:SER:HA	1:B:3110:GLN:NE2	2.24	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: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:A:837:GLU:O	1:A:838:ARG:CB	2.61	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:CE3	1:B:3140:TRP:HA	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:B:2964:TRP:HZ2	1:B:2966:ARG:HH11	1.59	0.48
1:A:1346:ILE:CD1	1:A:1362:ILE:HD11	2.43	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:1328:GLN:HE22	1:A:1364:ARG:HH11	1.61	0.48
1:A:761:THR:HB	1:A:766:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:ALA:HB2	1:A:1060:VAL:CG2	2.44	0.48
1:A:784:LYS:HD2	1:A:784:LYS:HA	1.59	0.48
1:B:3299:ALA:O	1:B:3304:VAL:HB	2.13	0.48
1:A:996:ARG:O	1:A:1017:LEU:HA	2.14	0.48
1:B:3324:GLN:HE22	5:B:2453:NAP:H2A	1.79	0.47
1:B:3247:VAL:HG11	1:B:3327:LEU:HD21	1.96	0.47
1:B:3053:ASP:HB3	1:B:3160:ALA:CB	2.45	0.47
1:A:1158:MET:CE	1:A:1159:PRO:HD2	2.44	0.47
1:A:1105:THR:OG1	1:A:1108:GLN:HG3	2.13	0.47
1:A:1110:GLN:HA	1:A:1110:GLN:HE21	1.78	0.47
1:B:3140:TRP:HE3	1:B:3140:TRP:HA	1.80	0.47
1:B:3057:ALA:HA	1:B:3090:ILE:HG22	1.96	0.47
1:B:3377:ALA:O	1:B:3381:ILE:HG13	2.15	0.47
1:B:3351:ASP:CB	1:B:3399:LEU:HG	2.44	0.47
1:A:1268:GLN:HE22	1:A:1302:LYS:HE2	1.80	0.47
1:A:1224:VAL:HG12	1:A:1224:VAL:O	2.14	0.47
1:A:1049:GLU:O	1:A:1049:GLU:HG3	2.15	0.47
1:A:947:ASP:N	1:A:947:ASP:OD1	2.48	0.47
1:A:1333:GLU:HA	1:A:1369:GLN:HE21	1.78	0.47
1:B:3379:VAL:O	1:B:3382:SER:HB3	2.15	0.46
1:B:2970:ARG:HD2	1:B:3079:TRP:CE3	2.49	0.46
1:A:876:ASN:C	1:A:876:ASN:ND2	2.64	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:3405:THR:O	1:B:3409:ARG:HG3	2.15	0.46
1:B:3362:ILE:O	1:B:3366:MET:HG2	2.15	0.46
1:B:3400:ARG:O	1:B:3404:VAL:HB	2.16	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: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:B:2902:LEU:HD23	1:B:2905:GLU:OE1	2.16	0.46
1:A:1059:HIS:O	1:A:1061:VAL:HG13	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:B:2889:TYR:CD1	1:B:3352:VAL:HG21	2.50	0.46
1:B:2884:LEU:N	1:B:2884:LEU:CD1	2.77	0.46
1:B:2787:SER:CB	1:B:2789:GLU:HG2	2.46	0.46
1:A:1049:GLU:O	1:A:1049:GLU:CG	2.64	0.46
1:B:2846:ASN:O	1:B:2891:HIS:CE1	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:GLU:O	1:A:877:VAL:HG22	2.16	0.46
1:A:1362:ILE:O	1:A:1366:MET:HG2	2.16	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:N	1:A:1317:ASP:OD1	2.46	0.45
1:B:2775:GLU:HA	1:B:2775:GLU:OE1	2.17	0.45
1:A:1309:TYR:CE1	1:A:1331:LEU:HD21	2.51	0.45
1:A:961:ASP:O	1:A:963:SER:N	2.48	0.45
1:B:3312:TYR:H	1:B:3321:LYS:HG3	1.82	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:A:762:GLU:HG3	1:A:809:PHE:CG	2.51	0.45
1:B:3132:LEU:O	1:B:3133:GLN:C	2.55	0.45
1:B:2755:ALA:HB2	1:B:2801:LEU:HD23	1.98	0.45
1:A:1372:LEU:HB3	1:A:1376:ASP:CB	2.41	0.45
1:B:3113:ALA:C	1:B:3115:LEU:H	2.19	0.45
1:B:2786:MET:SD	1:B:2791:TYR:HB2	2.57	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:OE1	1:B:3026:GLN:HA	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:B:3380:PHE:CD1	1:B:3380:PHE:C	2.90	0.45
1:A:787:SER:OG	1:A:789:GLU:HG2	2.16	0.45
1:B:3112:PHE:HZ	1:B:3146:MET:HE3	1.82	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:875:ALA:HA	1:A:907:GLY:O	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:841:TYR:HE2	1:A:846:ASN:ND2	2.16	0.44
5:A:1453:NAP:O3D	5:A:1453:NAP:PA	2.70	0.44
1:B:2971:LEU:CD2	1:B:3063:VAL:HG22	2.48	0.44
1:A:1351:ASP:CB	1:A:1399:LEU:HG	2.47	0.44
1:B:2769:TYR:CD2	1:B:2884:LEU:HD21	2.52	0.44
1:A:1061:VAL:O	1:A:1061:VAL:HG23	2.18	0.44
1:A:1050:ARG:O	1:A:1050:ARG:HD2	2.17	0.44
1:B:2961:ASP:C	1:B:2963:SER:H	2.21	0.44
1:B:3360:LYS:HB3	1:B:3364:ARG:CZ	2.44	0.44
1:B:3062:LYS:HD2	1:B:3081:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3053:ASP:HB3	1:B:3160:ALA:HB2	1.99	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:3134:GLU:OE1	1:B:3134:GLU:HA	2.18	0.44
1:B:3330:GLN:HB2	1:B:3331:LEU:HD12	1.98	0.44
1:A:830:HIS:NE2	1:A:838:ARG:O	2.34	0.44
1:B:3201:ASP:HB2	1:B:3402:TYR:OH	2.18	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:B:3193:ALA:CB	5:B:2453:NAP:C5D	2.95	0.43
1:B:2928:ARG:HH12	1:B:3130:LYS:HA	1.82	0.43
1:A:1089:THR:HG23	1:A:1092:GLN:OE1	2.18	0.43
1:A:841:TYR:CE2	1:A:846:ASN:ND2	2.86	0.43
1:B:3359:LEU:HD23	1:B:3359:LEU:C	2.38	0.43
1:A:1249:PRO:HG3	1:A:1354:MET:HG3	2.00	0.43
1:A:1331:LEU:O	1:A:1332:ALA:C	2.56	0.43
1:A:1027:TYR:CE1	1:A:1177:ILE:HG21	2.53	0.43
1:B:3110:GLN:CG	1:B:3111:GLN:N	2.81	0.43
1:A:1142:LYS:O	1:A:1143:ASN:C	2.56	0.43
1:B:3078:ASN:HB2	1:B:3080:LYS:HZ3	1.82	0.43
1:B:2882:PHE:CD1	1:B:2915:ARG:HB3	2.53	0.43
1:A:1132:LEU:O	1:A:1136:GLU:HG2	2.18	0.43
1:A:889:TYR:CD1	1:A:1352:VAL:HG21	2.54	0.43
1:B:3242:VAL:CG1	1:B:3343:GLY:O	2.65	0.43
1:A:813:ASP:HB3	1:A:814:PRO:CD	2.49	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:B:3158:MET:HE2	1:B:3159:PRO:O	2.18	0.43
1:A:1242:VAL:HG22	1:A:1243:PRO:HD2	2.00	0.43
1:A:961:ASP:CG	1:A:962:ARG:N	2.72	0.43
1:A:779:HIS:HB3	1:A:948:VAL:HG22	2.01	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:B:2912:LEU:HD23	1:B:2930:TRP:CD1	2.55	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:3019:THR:HG22	1:B:3022:ASN:CB	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3003:LEU:HD21	1:B:3014:PHE:HB2	2.02	0.42
1:A:1143:ASN:N	1:A:1144:PRO:CD	2.82	0.42
1:A:1134:GLU:CD	1:A:1134:GLU:H	2.23	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:1343:GLY:HA2	1:A:1389:ARG:NH2	2.34	0.42
1:A:762:GLU:HG3	1:A:809:PHE:CD1	2.55	0.42
1:B:2789:GLU:C	1:B:2791:TYR:H	2.23	0.42
1:A:936:LYS:HD2	1:A:936:LYS:HA	1.86	0.42
1:B:3130:LYS:O	1:B:3132:LEU:HG	2.19	0.42
1:B:3050:ARG:O	1:B:3050:ARG:HG3	2.18	0.42
1:B:2823:CYS:HA	1:B:2826:MET:HB2	2.02	0.42
1:A:1195:VAL:HA	5:A:1453:NAP:H5N	2.01	0.42
1:B:3401:THR:O	1:B:3405:THR:HB	2.20	0.42
1:B:3121:GLU:O	1:B:3125:LEU:HG	2.20	0.42
1:B:3309:TYR:CE1	1:B:3331:LEU:HD21	2.55	0.42
1:A:904:GLU:OE2	1:A:910:ARG:NH2	2.50	0.42
1:B:3409:ARG:O	1:B:3413:ILE:HG13	2.19	0.42
1:A:985:SER:HA	1:A:990:LYS:O	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:B:3257:ARG:HA	1:B:3260:TRP:CD2	2.55	0.41
1:A:784:LYS:HG2	1:B:2976:GLU:OE1	2.21	0.41
1:B:2779:HIS:HB2	1:B:2935:PHE:HZ	1.86	0.41
1:A:901:THR:O	1:A:905:GLU:HG3	2.20	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: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: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:3146:MET:HE2	1:B:3167:LEU:HD21	2.01	0.41
1:A:1318:ARG:CB	1:A:1319:PRO:CD	2.98	0.41
1:A:998:LEU:HD21	1:A:1018:HIS:HB2	2.01	0.41
1:B:3109:LEU:O	1:B:3112:PHE:N	2.54	0.41
1:A:996:ARG:HG3	6:A:5035:HOH:O	2.19	0.41
1:B:3040:HIS:O	1:B:3044:VAL:HG23	2.20	0.41
1:B:3371:LYS:HA	1:B:3371:LYS:HD3	1.62	0.41
1:A:1054:ALA:HB2	1:A:1160:ALA:HB2	2.01	0.41
1:B:2912:LEU:CD2	1:B:2934:VAL:CG2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:GLY:HA2	6:A:5051:HOH:O	2.20	0.41
1:A:1324:GLN:CG	1:A:1357:ASP:HB3	2.45	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:B:2828:MET:HG2	1:B:2906:LEU:HD22	2.01	0.41
1:B:3353:THR:CG2	5:B:2453:NAP:N6A	2.80	0.41
1:B:2843:VAL:HG12	1:B:2844:ARG:N	2.36	0.41
1:B:2788:MET:HE2	1:B:2821:PHE:HB3	2.02	0.41
1:A:935:PHE:CE2	1:A:948:VAL:HG11	2.56	0.41
1:A:780:ALA:N	1:A:948:VAL:HG21	2.35	0.41
1:B:2793:ILE:HD13	1:B:2824:ALA:CB	2.51	0.41
1:A:979:ASP:OD1	1:A:980:LEU:N	2.54	0.41
1:A:1263:ARG:HD3	1:A:1263:ARG:HA	1.81	0.41
1:B:3158:MET:HA	1:B:3159:PRO:HD3	1.85	0.41
1:B:2773:LEU:O	1:B:2776:ILE:CG2	2.69	0.41
1:B:3347:TYR:CZ	1:B:3391:HIS:CD2	3.09	0.41
1:A:1013:ILE:HD13	1:A:1194:ILE:HD11	2.04	0.40
1:B:3109:LEU:O	1:B:3110:GLN:C	2.60	0.40
1:B:2928:ARG:O	1:B:2931:ALA:HB3	2.21	0.40
1:A:762:GLU:HG2	1:A:815:PRO:HB3	2.04	0.40
1:A:946:ASP:OD1	1:A:946:ASP:C	2.60	0.40
1:B:3266:ASP:HB3	1:B:3272:MET:HG3	2.02	0.40
1:A:1183:MET:HG2	1:A:1184:TYR:CE2	2.56	0.40
1:A:982:GLN:OE1	1:A:982:GLN:HA	2.20	0.40
1:B:3332:ALA:HB1	1:B:3365:ILE:HG23	2.02	0.40
1:A:1328:GLN:HE21	1:A:1361:ALA:CB	2.31	0.40
1:A:1024:GLU:HA	1:A:1024:GLU:OE1	2.22	0.40
1:A:1317:ASP:C	1:A:1318:ARG:HG2	2.42	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:B:3055:PRO:O	1:B:3056:PRO:C	2.60	0.40
1:A:983:GLY:O	1:A:987:VAL:HG23	2.22	0.40
1:B:3062:LYS:HD2	1:B:3081:ASP:CG	2.42	0.40
1:B:2756:THR:HG22	1:B:2758:LEU:HG	2.03	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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	622/688 (90%)	569 (92%)	40 (6%)	13 (2%)	9	7
1	B	608/688 (88%)	548 (90%)	51 (8%)	9 (2%)	13	12
All	All	1230/1376 (89%)	1117 (91%)	91 (7%)	22 (2%)	11	9

All (22) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	543/601 (90%)	506 (93%)	37 (7%)	20	25
1	B	531/601 (88%)	496 (93%)	35 (7%)	21	27
All	All	1074/1202 (89%)	1002 (93%)	72 (7%)	20	26

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

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

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

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

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

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

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Mol	Chain	Res	Type
1	B	3261	GLN
1	B	3262	GLN
1	B	3324	GLN
1	B	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 carbohydrates 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FMN	A	1451	-	32,33,33	4.46	20 (62%)	34,50,50	3.50	11 (32%)
4	FAD	A	1452	-	52,58,58	5.38	38 (73%)	52,89,89	4.30	26 (50%)
5	NAP	A	1453	-	45,52,52	1.72	9 (20%)	55,80,80	2.13	12 (21%)
2	SO3	A	1500	-	1,3,3	2.72	1 (100%)	0,3,3	0.00	-
3	FMN	B	2451	-	32,33,33	4.65	19 (59%)	34,50,50	3.39	11 (32%)
4	FAD	B	2452	-	52,58,58	5.40	37 (71%)	52,89,89	4.39	23 (44%)
5	NAP	B	2453	-	45,52,52	2.60	9 (20%)	55,80,80	2.65	16 (29%)
2	SO3	B	2500	-	1,3,3	2.68	1 (100%)	0,3,3	0.00	-

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	A	1451	-	-	0/18/18/18	0/3/3/3
4	FAD	A	1452	-	-	0/30/50/50	0/6/6/6
5	NAP	A	1453	-	-	0/27/67/67	0/5/5/5
2	SO3	A	1500	-	-	0/0/0/0	0/0/0/0
3	FMN	B	2451	-	-	0/18/18/18	0/3/3/3
4	FAD	B	2452	-	-	0/30/50/50	0/6/6/6
5	NAP	B	2453	-	-	0/27/67/67	0/5/5/5
2	SO3	B	2500	-	-	0/0/0/0	0/0/0/0

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2452	FAD	C2B-C1B	-14.04	1.31	1.53
4	A	1452	FAD	C2B-C1B	-13.70	1.31	1.53
5	B	2453	NAP	C2D-C1D	-9.78	1.38	1.53
4	B	2452	FAD	C8A-N7A	-8.36	1.18	1.34
4	A	1452	FAD	C8A-N7A	-8.14	1.19	1.34
4	B	2452	FAD	C4'-C3'	-7.11	1.39	1.53
4	A	1452	FAD	P-O2P	-6.78	1.26	1.55
4	B	2452	FAD	P-O2P	-6.46	1.27	1.55
4	A	1452	FAD	PA-O2A	-6.45	1.27	1.55
4	A	1452	FAD	C4'-C3'	-6.35	1.40	1.53
4	B	2452	FAD	PA-O2A	-6.28	1.28	1.55
4	A	1452	FAD	C3B-C4B	-6.02	1.36	1.53
3	B	2451	FMN	C2'-C3'	-5.65	1.42	1.53
3	A	1451	FMN	C2'-C3'	-5.63	1.42	1.53
4	B	2452	FAD	C3B-C4B	-5.50	1.38	1.53
4	A	1452	FAD	C8M-C8	-5.02	1.41	1.51
4	B	2452	FAD	O2'-C2'	-5.00	1.32	1.43
3	A	1451	FMN	C1'-N10	-4.96	1.43	1.48
5	A	1453	NAP	C2D-C1D	-4.66	1.46	1.53
4	A	1452	FAD	O2'-C2'	-4.60	1.33	1.43
4	A	1452	FAD	O4-C4	-4.49	1.13	1.24
4	B	2452	FAD	P-O1P	-4.48	1.34	1.51
4	A	1452	FAD	O5'-C5'	-4.47	1.27	1.44
4	A	1452	FAD	C6-C5X	-4.26	1.35	1.41
4	B	2452	FAD	C8M-C8	-4.24	1.42	1.51
4	A	1452	FAD	P-O1P	-4.13	1.36	1.51
4	A	1452	FAD	O3B-C3B	-3.92	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2452	FAD	O4-C4	-3.90	1.14	1.24
3	B	2451	FMN	C1'-N10	-3.78	1.44	1.48
4	B	2452	FAD	O3B-C3B	-3.71	1.34	1.43
4	B	2452	FAD	PA-O1A	-3.67	1.37	1.51
4	B	2452	FAD	O5'-C5'	-3.66	1.30	1.44
3	A	1451	FMN	C4-C4A	-3.61	1.33	1.41
3	B	2451	FMN	O2'-C2'	-3.52	1.35	1.43
3	A	1451	FMN	O2'-C2'	-3.51	1.35	1.43
4	A	1452	FAD	PA-O1A	-3.29	1.39	1.51
4	A	1452	FAD	C5A-N7A	-2.95	1.28	1.39
3	B	2451	FMN	C4-C4A	-2.79	1.35	1.41
3	A	1451	FMN	P-O1P	-2.79	1.42	1.50
4	B	2452	FAD	C5A-N7A	-2.75	1.29	1.39
5	B	2453	NAP	C2N-C3N	-2.74	1.34	1.39
3	B	2451	FMN	P-O3P	-2.65	1.45	1.54
5	A	1453	NAP	C2D-C3D	-2.56	1.46	1.53
3	B	2451	FMN	P-O1P	-2.42	1.43	1.50
4	B	2452	FAD	C6-C5X	-2.40	1.38	1.41
3	A	1451	FMN	P-O3P	-2.33	1.46	1.54
3	A	1451	FMN	C7M-C7	-2.21	1.46	1.51
4	A	1452	FAD	C2B-C3B	-2.11	1.47	1.53
5	A	1453	NAP	P2B-O2X	-2.11	1.47	1.54
5	B	2453	NAP	PN-O2N	-2.01	1.46	1.55
4	B	2452	FAD	C5A-C4A	2.05	1.45	1.40
4	A	1452	FAD	C6A-N6A	2.22	1.43	1.34
4	A	1452	FAD	C5A-C4A	2.32	1.45	1.40
4	A	1452	FAD	C5X-N5	2.36	1.39	1.35
4	A	1452	FAD	O3'-C3'	2.41	1.48	1.43
4	A	1452	FAD	C1'-C2'	2.46	1.67	1.51
5	A	1453	NAP	C3N-C7N	2.47	1.54	1.50
5	A	1453	NAP	C4N-C3N	2.49	1.43	1.39
5	B	2453	NAP	O3D-C3D	2.55	1.49	1.43
4	B	2452	FAD	C6A-N6A	2.59	1.44	1.34
2	B	2500	SO3	O1-S	2.68	1.54	1.44
4	A	1452	FAD	C6A-C5A	2.70	1.56	1.42
4	B	2452	FAD	C1'-C2'	2.70	1.68	1.51
2	A	1500	SO3	O1-S	2.72	1.55	1.44
4	B	2452	FAD	C6A-C5A	2.76	1.57	1.42
3	B	2451	FMN	C6-C5A	2.88	1.46	1.41
5	B	2453	NAP	O4B-C1B	2.88	1.45	1.41
3	A	1451	FMN	C6-C5A	3.04	1.46	1.41
4	B	2452	FAD	C5B-C4B	3.11	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1453	NAP	O4D-C1D	3.12	1.45	1.41
5	A	1453	NAP	O4B-C1B	3.12	1.45	1.41
5	A	1453	NAP	C6N-N1N	3.18	1.44	1.35
3	B	2451	FMN	C5'-C4'	3.25	1.56	1.51
4	A	1452	FAD	O4B-C1B	3.38	1.46	1.41
3	A	1451	FMN	C5'-C4'	3.47	1.57	1.51
4	B	2452	FAD	C9A-N10	3.53	1.43	1.38
4	A	1452	FAD	C10-N1	3.57	1.41	1.35
5	B	2453	NAP	C4N-C3N	3.58	1.45	1.39
5	B	2453	NAP	C6N-N1N	3.61	1.45	1.35
4	B	2452	FAD	C5X-N5	3.61	1.41	1.35
4	B	2452	FAD	C10-N1	3.84	1.42	1.35
4	B	2452	FAD	O3'-C3'	3.90	1.52	1.43
4	A	1452	FAD	C5B-C4B	3.99	1.64	1.51
4	B	2452	FAD	C2'-C3'	4.05	1.61	1.53
4	A	1452	FAD	C9A-N10	4.09	1.44	1.38
3	B	2451	FMN	O3'-C3'	4.12	1.52	1.43
3	B	2451	FMN	C6-C7	4.14	1.49	1.37
4	A	1452	FAD	C9-C9A	4.17	1.49	1.40
4	B	2452	FAD	C9-C9A	4.19	1.49	1.40
4	B	2452	FAD	O4B-C1B	4.22	1.47	1.41
3	A	1451	FMN	C6-C7	4.45	1.50	1.37
3	B	2451	FMN	C8-C7	4.45	1.52	1.41
3	A	1451	FMN	O3'-C3'	4.47	1.53	1.43
3	A	1451	FMN	C8-C7	4.47	1.53	1.41
3	A	1451	FMN	C9A-C5A	4.54	1.52	1.42
3	A	1451	FMN	C2-N3	4.67	1.47	1.38
4	B	2452	FAD	C4X-N5	4.74	1.40	1.33
3	B	2451	FMN	C9A-C5A	5.34	1.53	1.42
3	B	2451	FMN	C2-N3	5.38	1.49	1.38
4	B	2452	FAD	C4-N3	5.38	1.42	1.33
4	A	1452	FAD	C2'-C3'	5.52	1.64	1.53
5	B	2453	NAP	O4D-C1D	5.59	1.49	1.41
4	A	1452	FAD	C4X-N5	5.77	1.42	1.33
4	A	1452	FAD	C4-N3	5.89	1.43	1.33
3	A	1451	FMN	C9A-N10	6.00	1.47	1.38
5	A	1453	NAP	C2N-N1N	6.14	1.43	1.35
4	B	2452	FAD	O4'-C4'	6.19	1.57	1.43
3	A	1451	FMN	C10-N10	6.22	1.46	1.39
3	B	2451	FMN	C10-N10	6.55	1.46	1.39
4	B	2452	FAD	C8-C7	6.61	1.58	1.41
4	A	1452	FAD	O4'-C4'	7.03	1.59	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2451	FMN	C9A-N10	7.20	1.49	1.38
4	A	1452	FAD	C10-N10	7.34	1.47	1.39
4	A	1452	FAD	C8-C7	7.41	1.60	1.41
4	B	2452	FAD	C9A-C5X	7.59	1.58	1.42
3	A	1451	FMN	C9-C9A	7.81	1.57	1.40
3	B	2451	FMN	C9-C9A	7.87	1.57	1.40
4	B	2452	FAD	C1'-N10	7.93	1.56	1.48
4	A	1452	FAD	C9A-C5X	8.29	1.60	1.42
3	B	2451	FMN	C5A-N5	8.72	1.49	1.35
3	A	1451	FMN	C5A-N5	9.09	1.49	1.35
3	A	1451	FMN	C4-N3	9.13	1.49	1.33
4	A	1452	FAD	C1'-N10	9.21	1.58	1.48
5	B	2453	NAP	C2N-N1N	9.33	1.48	1.35
4	A	1452	FAD	C2A-N3A	9.83	1.49	1.32
3	A	1451	FMN	C4A-C10	9.92	1.59	1.40
4	B	2452	FAD	C2A-N3A	10.06	1.50	1.32
3	B	2451	FMN	C4-N3	10.31	1.51	1.33
4	B	2452	FAD	C10-N10	10.34	1.51	1.39
4	A	1452	FAD	C2A-N1A	10.93	1.55	1.33
4	B	2452	FAD	C2A-N1A	11.27	1.55	1.33
3	B	2451	FMN	C4A-C10	11.39	1.61	1.40
4	A	1452	FAD	C4A-N3A	13.48	1.55	1.35
4	B	2452	FAD	C4A-N3A	14.43	1.56	1.35

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2452	FAD	O4B-C1B-N9A	-15.67	78.51	108.11
4	A	1452	FAD	O4B-C1B-N9A	-15.46	78.90	108.11
4	A	1452	FAD	C1B-N9A-C4A	-11.37	114.12	126.81
4	B	2452	FAD	N3A-C2A-N1A	-11.06	120.18	128.87
4	B	2452	FAD	C1B-N9A-C4A	-11.04	114.48	126.81
4	A	1452	FAD	N3A-C2A-N1A	-10.32	120.77	128.87
5	B	2453	NAP	N3A-C2A-N1A	-10.21	120.85	128.87
5	A	1453	NAP	N3A-C2A-N1A	-9.65	121.29	128.87
4	A	1452	FAD	C5X-C9A-N10	-8.39	111.29	117.58
4	B	2452	FAD	C5X-C9A-N10	-8.19	111.44	117.58
5	B	2453	NAP	C4D-O4D-C1D	-8.14	101.02	109.64
3	A	1451	FMN	N3-C2-N1	-7.60	114.89	127.69
3	B	2451	FMN	N3-C2-N1	-7.34	115.33	127.69
5	A	1453	NAP	C4D-O4D-C1D	-6.88	102.35	109.64
4	B	2452	FAD	C4X-C10-N10	-6.00	116.16	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2452	FAD	N3-C2-N1	-5.97	117.63	127.69
4	A	1452	FAD	N3-C2-N1	-5.84	117.86	127.69
4	A	1452	FAD	C4X-C10-N10	-5.51	116.52	120.52
4	B	2452	FAD	O5'-P-O1P	-5.48	86.79	109.21
4	A	1452	FAD	O5'-P-O1P	-5.45	86.89	109.21
3	A	1451	FMN	C4A-C4-N3	-5.01	116.97	123.52
3	B	2451	FMN	C4A-C4-N3	-4.92	117.10	123.52
3	A	1451	FMN	C7M-C7-C6	-4.39	107.92	120.33
3	B	2451	FMN	C7M-C7-C6	-4.37	107.98	120.33
4	B	2452	FAD	O5B-PA-O1A	-4.16	92.19	109.21
4	A	1452	FAD	O5B-PA-O1A	-3.56	94.63	109.21
4	B	2452	FAD	C4X-C4-N3	-3.52	118.92	123.52
4	A	1452	FAD	O4B-C4B-C3B	-3.44	98.18	105.16
3	A	1451	FMN	C9A-C5A-N5	-3.33	116.76	122.18
3	B	2451	FMN	C9A-C5A-N5	-3.13	117.08	122.18
5	B	2453	NAP	O7N-C7N-C3N	-3.02	116.25	119.60
4	A	1452	FAD	C4X-C4-N3	-3.00	119.60	123.52
4	B	2452	FAD	O4B-C4B-C5B	-2.89	98.95	109.29
4	B	2452	FAD	O3'-C3'-C2'	-2.76	101.57	108.73
4	B	2452	FAD	O4B-C4B-C3B	-2.71	99.67	105.16
5	B	2453	NAP	C5D-C4D-C3D	-2.69	104.80	115.20
4	A	1452	FAD	O4B-C4B-C5B	-2.67	99.73	109.29
4	A	1452	FAD	O3'-C3'-C2'	-2.62	101.92	108.73
5	B	2453	NAP	O5B-C5B-C4B	-2.42	100.38	109.09
5	A	1453	NAP	O4B-C4B-C5B	-2.40	100.69	109.29
4	B	2452	FAD	C4-C4X-N5	-2.33	115.86	118.70
5	B	2453	NAP	C3N-C2N-N1N	-2.31	117.70	120.34
5	A	1453	NAP	O5B-C5B-C4B	-2.26	100.92	109.09
5	A	1453	NAP	O7N-C7N-C3N	-2.23	117.12	119.60
4	A	1452	FAD	C4-C4X-N5	-2.22	115.99	118.70
5	A	1453	NAP	C5D-C4D-C3D	-2.22	106.60	115.20
5	B	2453	NAP	C2D-C3D-C4D	-2.22	98.09	102.64
4	A	1452	FAD	C4B-O4B-C1B	-2.22	107.29	109.64
4	A	1452	FAD	C7M-C7-C6	-2.13	114.32	120.33
5	B	2453	NAP	C2D-C1D-N1N	-2.13	109.37	113.53
4	A	1452	FAD	C4-C4X-C10	-2.06	118.62	119.94
4	B	2452	FAD	O4'-C4'-C5'	-2.05	105.63	110.09
4	B	2452	FAD	C8M-C8-C9	-2.01	114.64	120.33
4	A	1452	FAD	O2P-P-O1P	2.05	123.22	112.56
5	A	1453	NAP	O3X-P2B-O2X	2.08	115.09	107.44
4	A	1452	FAD	C4X-N5-C5X	2.10	119.20	116.72
4	A	1452	FAD	C7M-C7-C8	2.14	125.32	120.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1452	FAD	C2B-C3B-C4B	2.16	107.05	102.64
5	A	1453	NAP	O2N-PN-O5D	2.21	118.79	108.24
5	B	2453	NAP	O2N-PN-O5D	2.26	118.99	108.24
4	A	1452	FAD	O2'-C2'-C1'	2.28	115.55	109.93
5	A	1453	NAP	C5N-C4N-C3N	2.31	123.11	120.35
5	B	2453	NAP	O3D-C3D-C2D	2.38	119.55	111.86
5	B	2453	NAP	O3X-P2B-O2X	2.55	116.82	107.44
4	B	2452	FAD	C2B-C3B-C4B	2.61	107.98	102.64
4	A	1452	FAD	C1'-C2'-C3'	2.67	117.44	109.82
4	B	2452	FAD	C4X-N5-C5X	2.73	119.94	116.72
5	B	2453	NAP	O3D-C3D-C4D	2.74	119.19	111.01
4	B	2452	FAD	C1'-C2'-C3'	2.81	117.87	109.82
4	B	2452	FAD	O2'-C2'-C1'	2.92	117.15	109.93
3	B	2451	FMN	C6-C5A-N5	3.18	122.87	118.92
5	A	1453	NAP	O4D-C1D-N1N	3.35	111.72	108.10
5	B	2453	NAP	C5N-C4N-C3N	3.41	124.42	120.35
3	A	1451	FMN	O3P-P-O2P	3.48	120.22	107.44
4	B	2452	FAD	C2A-N1A-C6A	3.51	125.04	118.77
5	A	1453	NAP	N6A-C6A-N1A	3.55	124.47	118.52
3	B	2451	FMN	O3P-P-O2P	3.59	120.64	107.44
3	A	1451	FMN	C6-C5A-N5	3.62	123.43	118.92
4	A	1452	FAD	C2A-N1A-C6A	3.69	125.36	118.77
5	B	2453	NAP	N6A-C6A-N1A	3.94	125.13	118.52
5	B	2453	NAP	O4B-C1B-N9A	4.07	115.79	108.11
5	A	1453	NAP	O4B-C1B-N9A	4.29	116.21	108.11
3	A	1451	FMN	C7M-C7-C8	4.38	130.15	120.73
3	B	2451	FMN	C7M-C7-C8	4.45	130.29	120.73
3	A	1451	FMN	C1'-N10-C9A	4.50	124.04	118.83
3	B	2451	FMN	C1'-N10-C9A	4.81	124.41	118.83
3	A	1451	FMN	C4A-N5-C5A	5.72	123.47	116.72
3	B	2451	FMN	C4A-N5-C5A	5.75	123.50	116.72
3	A	1451	FMN	C5A-C9A-N10	6.70	122.60	117.58
3	B	2451	FMN	C5A-C9A-N10	6.83	122.69	117.58
4	A	1452	FAD	C2B-C1B-N9A	7.39	133.26	113.47
4	A	1452	FAD	C4-N3-C2	7.58	121.48	115.16
4	B	2452	FAD	C2B-C1B-N9A	7.71	134.11	113.47
5	B	2453	NAP	O4D-C1D-N1N	8.00	116.74	108.10
4	B	2452	FAD	C4-N3-C2	8.36	122.13	115.16
4	B	2452	FAD	O2A-PA-O3P	8.82	143.06	105.27
4	A	1452	FAD	O2A-PA-O3P	9.00	143.82	105.27
3	B	2451	FMN	C4-N3-C2	10.53	123.94	115.16
3	A	1451	FMN	C4-N3-C2	11.30	124.59	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1453	NAP	9	0
5	B	2453	NAP	13	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	630/688 (91%)	0.61	52 (8%) 14 20	28, 52, 88, 99	0
1	B	616/688 (89%)	0.84	83 (13%) 4 6	24, 61, 93, 100	0
All	All	1246/1376 (90%)	0.72	135 (10%) 8 11	24, 56, 92, 100	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	830	HIS	9.9
1	B	2902	LEU	8.8
1	B	3316	PRO	7.9
1	B	2845	PHE	7.5
1	A	950	ILE	7.2
1	B	3413	ILE	7.1
1	B	2843	VAL	6.9
1	B	2948	VAL	6.0
1	A	948	VAL	5.9
1	B	3371	LYS	5.7
1	A	1073	LEU	5.6
1	B	2967	ASN	5.6
1	B	3073	LEU	5.4
1	B	3411	GLU	5.2
1	A	1413	ILE	5.0
1	B	2794	VAL	4.8
1	B	2947	ASP	4.7
1	B	2906	LEU	4.7
1	B	2752	ARG	4.6
1	B	3402	TYR	4.6
1	A	838	ARG	4.5
1	A	1057	ALA	4.5
1	B	2779	HIS	4.4
1	B	2949	ASN	4.3

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

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Mol	Chain	Res	Type	RSRZ
1	B	2842	LYS	2.9
1	A	1117	THR	2.9
1	B	2796	LEU	2.9
1	B	2905	GLU	2.9
1	A	1375	GLU	2.8
1	B	2828	MET	2.8
1	A	1121	GLU	2.8
1	B	2844	ARG	2.7
1	A	1254	ALA	2.7
1	A	1318	ARG	2.7
1	B	3072	ALA	2.7
1	B	2920	LEU	2.7
1	A	945	GLY	2.6
1	B	2819	GLU	2.6
1	B	2827	GLU	2.6
1	A	1119	GLU	2.6
1	B	3120	LYS	2.6
1	B	2915	ARG	2.5
1	A	1132	LEU	2.5
1	A	1364	ARG	2.5
1	A	1076	ILE	2.5
1	B	3253	ILE	2.5
1	A	847	SER	2.5
1	B	2765	LYS	2.5
1	B	3376	ASP	2.5
1	B	2753	VAL	2.5
1	B	3140	TRP	2.5
1	B	2841	TYR	2.5
1	B	3119	GLU	2.5
1	B	2766	SER	2.4
1	B	3383	ARG	2.4
1	A	1054	ALA	2.4
1	A	1120	LYS	2.4
1	A	751	LYS	2.4
1	A	846	ASN	2.4
1	B	3127	VAL	2.3
1	B	3378	GLY	2.3
1	A	1058	ASN	2.3
1	A	1403	GLU	2.2
1	B	3285	GLN	2.2
1	B	3246	LEU	2.2
1	B	3201	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	976	GLU	2.2
1	B	2950	ILE	2.2
1	B	2903	LEU	2.2
1	A	964	TRP	2.2
1	B	3068	GLU	2.2
1	A	1130	LYS	2.2
1	B	3287	LYS	2.2
1	A	1246	LEU	2.2
1	A	1280	VAL	2.2
1	B	3130	LYS	2.2
1	B	3066	LEU	2.2
1	A	963	SER	2.2
1	B	3349	CYS	2.1
1	B	3116	ALA	2.1
1	B	2976	GLU	2.1
1	B	2817	ASN	2.1
1	A	960	ASN	2.1
1	B	2789	GLU	2.1
1	A	1175	TYR	2.1
1	A	1072	ALA	2.1
1	B	3379	VAL	2.1
1	B	3377	ALA	2.0
1	B	2946	ASP	2.0
1	A	1407	ARG	2.0
1	B	3053	ASP	2.0
1	B	3058	ASN	2.0
1	B	3176	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAP	B	2453	48/48	0.87	0.18	0.54	40,47,59,61	0
5	NAP	A	1453	48/48	0.92	0.17	0.38	27,44,54,56	0
3	FMN	A	1451	31/31	0.96	0.17	0.10	32,35,38,41	0
4	FAD	A	1452	53/53	0.97	0.17	-0.21	17,30,51,53	0
2	SO3	B	2500	4/4	0.92	0.13	-0.23	79,80,81,82	0
4	FAD	B	2452	53/53	0.96	0.16	-0.44	17,29,59,59	0
3	FMN	B	2451	31/31	0.96	0.18	-0.54	45,49,53,54	0
2	SO3	A	1500	4/4	0.83	0.22	-	67,68,68,68	4

6.5 Other polymers [i](#)

There are no such residues in this entry.