



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 08:08 pm GMT

PDB ID : 2WP5
Title : Trypanosoma brucei trypanothione reductase in complex with 3,4- dihydro-quinazoline inhibitor (DDD00065414)
Authors : Alphey, M.S.; Patterson, S.; Fairlamb, A.H.
Deposited on : 2009-08-03
Resolution : 2.80 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

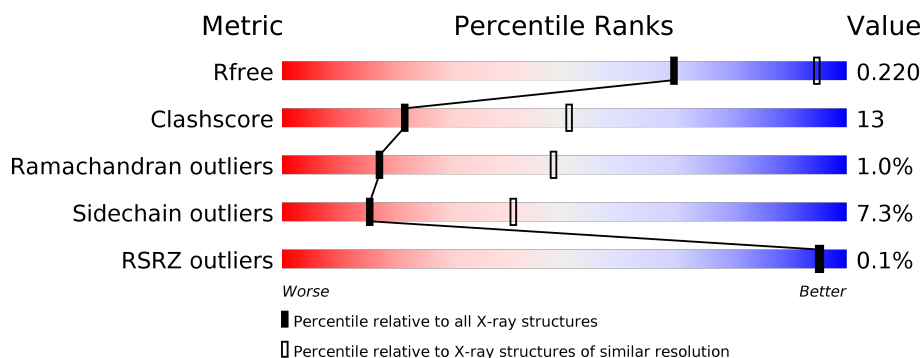
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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	495	
1	B	495	
1	C	495	
1	D	495	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MRD	A	1491	-	-	X	-
7	MPD	D	1491	-	-	X	-
7	MPD	D	1492	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15423 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.

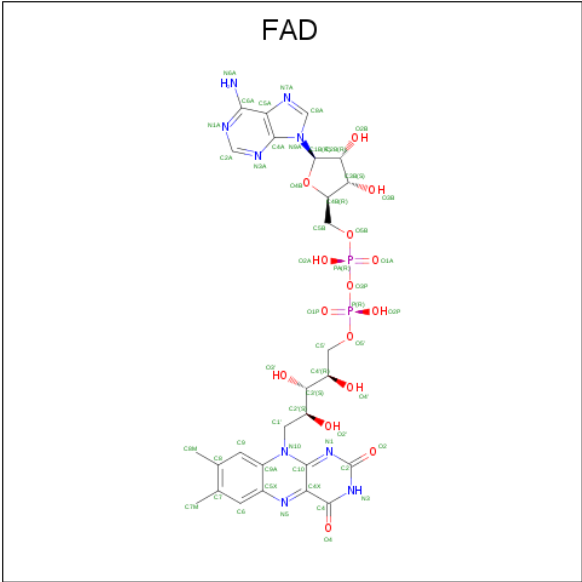
- Molecule 1 is a protein called TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	2	0
			3735	2380	634	701	20			
1	B	485	Total	C	N	O	S	0	5	0
			3715	2363	635	698	19			
1	C	485	Total	C	N	O	S	0	2	0
			3700	2355	629	697	19			
1	D	488	Total	C	N	O	S	0	1	0
			3716	2364	631	701	20			

There are 12 discrepancies between the modelled and reference sequences:

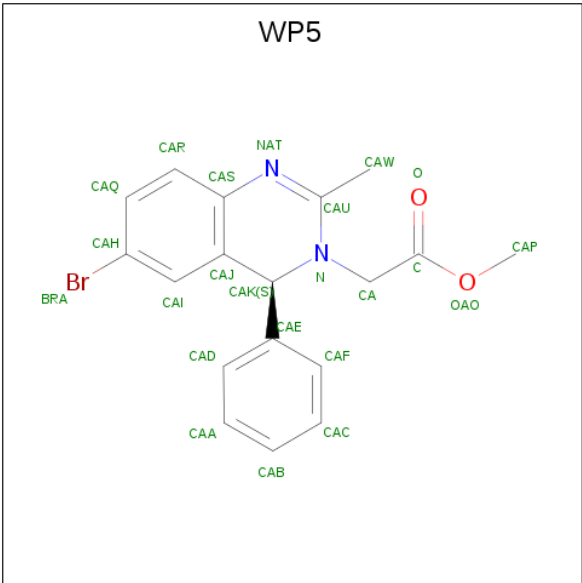
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q389T8
A	-1	SER	-	expression tag	UNP Q389T8
A	0	HIS	-	expression tag	UNP Q389T8
B	-2	GLY	-	expression tag	UNP Q389T8
B	-1	SER	-	expression tag	UNP Q389T8
B	0	HIS	-	expression tag	UNP Q389T8
C	-2	GLY	-	expression tag	UNP Q389T8
C	-1	SER	-	expression tag	UNP Q389T8
C	0	HIS	-	expression tag	UNP Q389T8
D	-2	GLY	-	expression tag	UNP Q389T8
D	-1	SER	-	expression tag	UNP Q389T8
D	0	HIS	-	expression tag	UNP Q389T8

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is METHYL [(4S)-6-BROMO-2-METHYL-4-PHENYLQUINAZOLIN-3(4H)-YL]ACETATE (three-letter code: WP5) (formula: C₁₈H₁₇BrN₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			23	1	18	2	2		
3	B	1	Total	Br	C	N	O	0	0
			23	1	18	2	2		
3	C	1	Total	Br	C	N	O	0	0
			23	1	18	2	2		
3	D	1	Total	Br	C	N	O	0	0
			23	1	18	2	2		

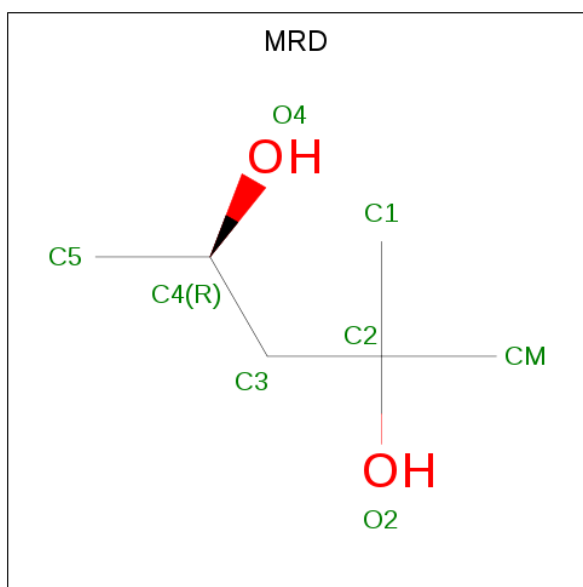
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		
4	A	2	Total	Cl	0	0
			2	2		
4	D	2	Total	Cl	0	0
			2	2		
4	C	2	Total	Cl	0	0
			2	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

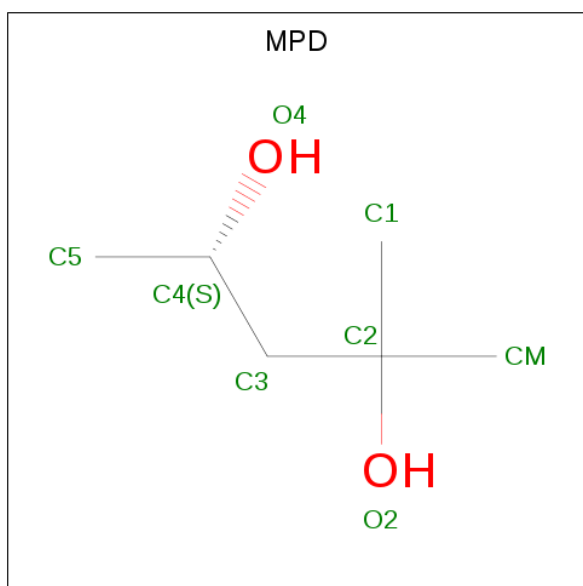
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	1	Total	Na	0	0
			1	1		
5	D	2	Total	Na	0	0
			2	2		
5	C	1	Total	Na	0	0
			1	1		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			8	6	2		

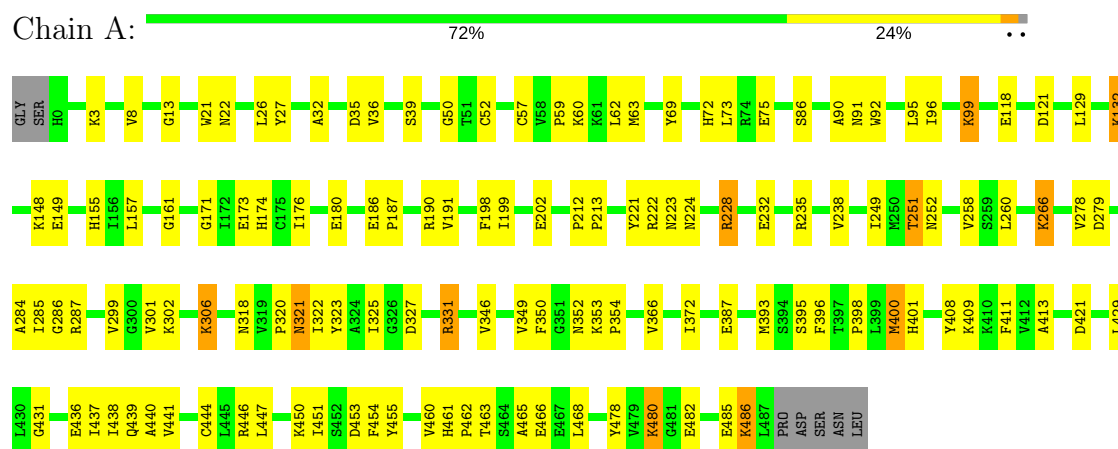
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	71	Total	O	0	0
			71	71		
8	B	44	Total	O	0	0
			44	44		
8	C	36	Total	O	0	0
			36	36		
8	D	56	Total	O	0	0
			56	56		

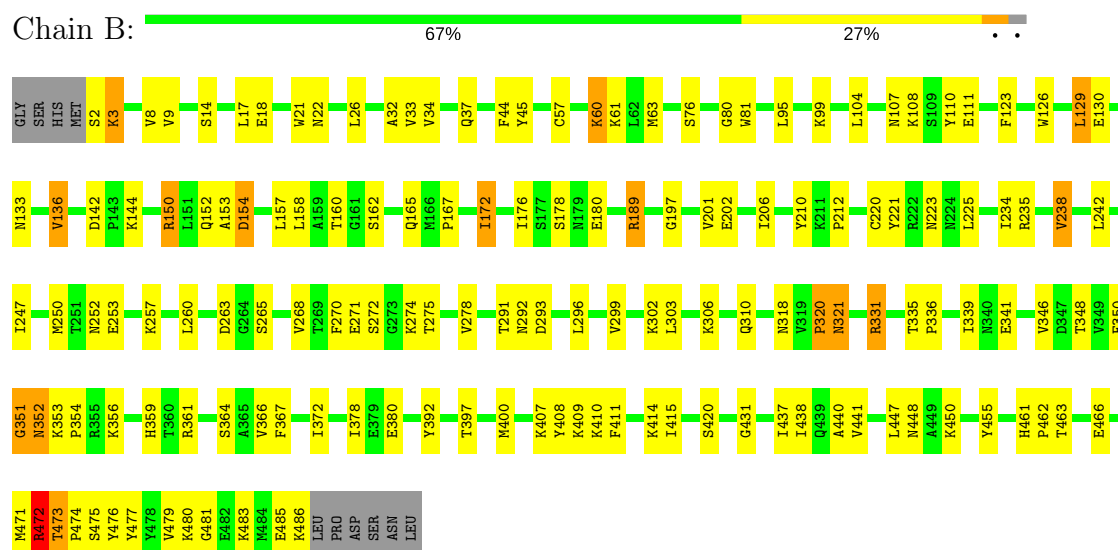
3 Residue-property plots

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

• Molecule 1: TRYPANOTHIONE REDUCTASE

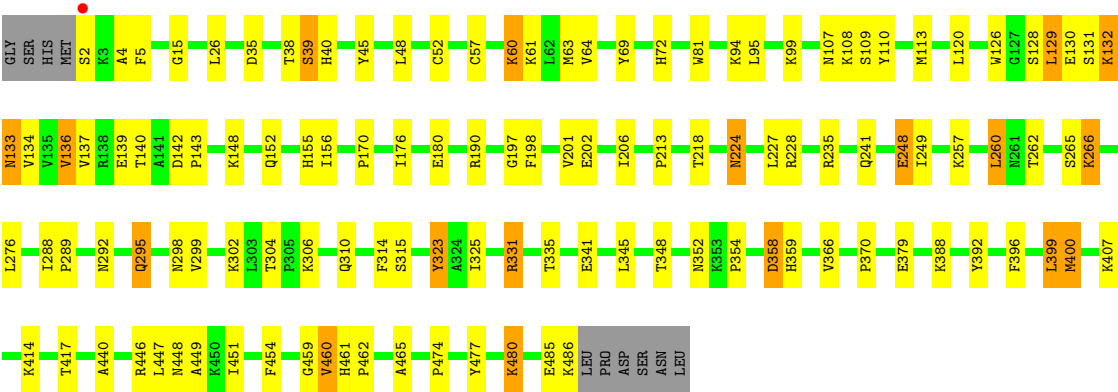


• Molecule 1: TRYPANOTHIONE REDUCTASE

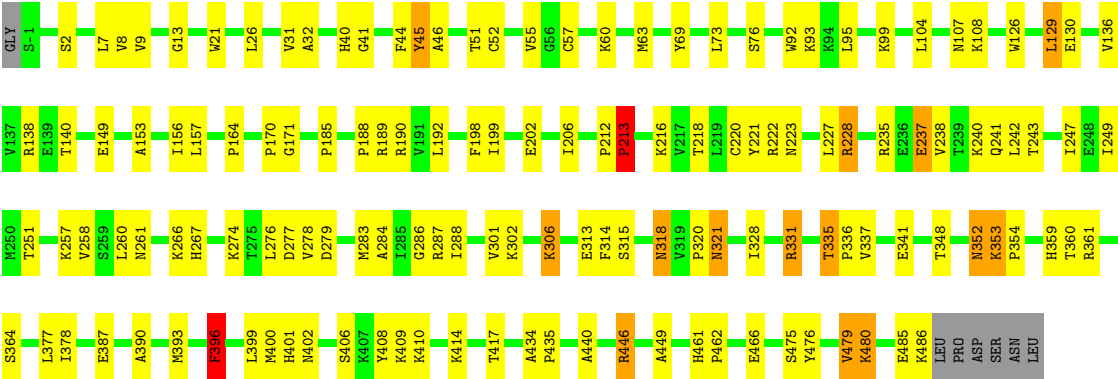


• Molecule 1: TRYPANOTHIONE REDUCTASE





● Molecule 1: TRYPANOTHIONE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.94Å 63.30Å 169.41Å 90.00° 98.09° 90.00°	Depositor
Resolution (Å)	46.71 – 2.80 46.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.71-2.80) 83.4 (46.71-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.164 , 0.219 0.165 , 0.220	Depositor DCC
R_{free} test set	2203 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15423	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, CL, WP5, NA, MRD, 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	0.84	2/3824 (0.1%)	0.84	1/5186 (0.0%)
1	B	0.78	0/3807	0.83	3/5161 (0.1%)
1	C	0.82	0/3784	0.84	5/5132 (0.1%)
1	D	0.84	1/3798 (0.0%)	0.88	3/5151 (0.1%)
All	All	0.82	3/15213 (0.0%)	0.85	12/20630 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	CYS	CB-SG	-5.86	1.72	1.81
1	D	228	ARG	CG-CD	5.68	1.66	1.51
1	A	321	ASN	CB-CG	5.18	1.62	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	26	LEU	CA-CB-CG	7.35	132.22	115.30
1	B	472	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	A	121	ASP	CB-CG-OD1	6.44	124.10	118.30
1	C	190	ARG	NE-CZ-NH2	-6.09	117.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	260	LEU	CA-CB-CG	5.90	128.87	115.30
1	C	358	ASP	CB-CG-OD1	5.57	123.32	118.30
1	B	361	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	C	276	LEU	CA-CB-CG	5.43	127.80	115.30
1	B	189	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	26	LEU	CA-CB-CG	5.12	127.07	115.30
1	C	260	LEU	CA-CB-CG	5.11	127.06	115.30
1	D	276	LEU	CB-CG-CD2	-5.02	102.47	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	351	GLY	Peptide
1	D	396	PHE	Peptide
1	D	479	VAL	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3735	0	3751	98	0
1	B	3715	0	3741	110	0
1	C	3700	0	3712	73	0
1	D	3716	0	3723	120	0
2	A	53	0	31	0	0
2	B	53	0	31	2	0
2	C	53	0	31	0	0
2	D	53	0	31	3	0
3	A	23	0	17	2	0
3	B	23	0	17	4	0
3	C	23	0	17	2	0
3	D	23	0	17	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
6	A	16	0	28	9	0
7	D	16	0	28	26	0
8	A	71	0	0	4	0
8	B	44	0	0	3	0
8	C	36	0	0	4	0
8	D	56	0	0	8	0
All	All	15423	0	15175	390	0

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 13.

All (390) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ALA:HA	6:A:1491:MRD:H5C2	1.19	1.08
1:B:234:ILE:O	1:B:238:VAL:HG12	1.55	1.06
1:C:348:THR:HB	8:C:2020:HOH:O	1.55	1.04
1:B:351:GLY:CA	1:B:352:ASN:HB2	1.86	1.03
1:D:485:GLU:HG2	1:D:485:GLU:O	1.60	1.02
1:A:284:ALA:HA	6:A:1491:MRD:C5	1.90	1.01
1:A:132:LYS:NZ	1:A:321:ASN:HB2	1.76	1.01
1:A:199:ILE:HD12	6:A:1491:MRD:H1C1	1.46	0.96
1:B:472:ARG:HH11	1:B:472:ARG:HG3	1.28	0.95
1:D:164:PRO:HB3	7:D:1491:MPD:H53	1.47	0.95
1:D:318:ASN:H	1:D:318:ASN:HD22	1.14	0.94
1:B:130:GLU:OE2	1:B:150:ARG:NH2	2.02	0.93
1:D:185:PRO:HD2	8:D:2025:HOH:O	1.72	0.90
1:C:130:GLU:HB2	1:C:136:VAL:HG22	1.53	0.90
1:A:485:GLU:HG3	1:A:486:LYS:HG2	1.53	0.88
1:B:351:GLY:HA3	1:B:352:ASN:HB2	1.53	0.88
1:A:21:TRP:CD1	3:A:1000:WP5:HAW3	2.09	0.88
1:A:387:GLU:OE1	1:A:480:LYS:HG2	1.75	0.86
1:D:286:GLY:N	7:D:1491:MPD:H11	1.90	0.85
1:D:199:ILE:HD12	7:D:1491:MPD:O2	1.76	0.85
1:B:448[B]:ASN:HD21	1:B:450:LYS:NZ	1.76	0.81
1:C:155:HIS:HD1	1:C:323:TYR:HH	1.25	0.80
1:D:284:ALA:HB1	7:D:1491:MPD:HM3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:PHE:H	1:D:396:PHE:HD1	1.30	0.79
1:A:132:LYS:HZ2	1:A:321:ASN:HB2	1.48	0.79
1:C:295:GLN:NE2	1:C:295:GLN:HA	1.97	0.78
1:D:377:LEU:HD23	7:D:1492:MPD:H11	1.66	0.77
1:B:302:LYS:H	1:B:318:ASN:HD21	1.32	0.77
1:A:228:ARG:NH1	1:A:235:ARG:HH22	1.83	0.77
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.67	0.77
1:D:192:LEU:HD11	1:D:220:CYS:SG	2.26	0.76
1:D:286:GLY:H	7:D:1491:MPD:H11	1.49	0.76
1:D:284:ALA:HA	7:D:1491:MPD:H52	1.68	0.75
1:B:8:VAL:HG22	1:B:32:ALA:HB3	1.67	0.75
1:A:132:LYS:HZ1	1:A:321:ASN:HB2	1.51	0.75
1:B:472:ARG:CG	1:B:472:ARG:HH11	2.00	0.74
1:B:37:GLN:OE1	1:B:44:PHE:HB2	1.87	0.73
1:A:3:LYS:NZ	1:A:149:GLU:OE1	2.15	0.73
1:B:250:MET:CE	1:B:253:GLU:HG3	2.18	0.73
1:A:224:ASN:HB3	1:A:252:ASN:HD21	1.54	0.72
1:B:129:LEU:HD23	1:B:299:VAL:HG21	1.70	0.72
1:D:321:ASN:CB	8:D:2014:HOH:O	2.38	0.71
1:B:302:LYS:HD3	1:B:310:GLN:HE22	1.56	0.70
1:B:351:GLY:HA2	1:B:352:ASN:HB2	1.71	0.70
1:D:284:ALA:HB1	7:D:1491:MPD:CM	2.21	0.70
1:D:286:GLY:CA	7:D:1491:MPD:H13	2.22	0.70
1:B:60:LYS:NZ	2:B:998:FAD:O4	2.25	0.70
1:A:132:LYS:NZ	1:A:321:ASN:CB	2.55	0.69
1:A:157:LEU:HD11	1:A:325:ILE:HG12	1.75	0.69
1:B:250:MET:HE2	1:B:253:GLU:HG3	1.75	0.69
1:A:221:TYR:CE2	1:A:223:ASN:HB2	2.27	0.69
1:A:22:ASN:O	1:A:26:LEU:HB2	1.93	0.69
1:D:286:GLY:N	7:D:1491:MPD:C1	2.54	0.69
1:A:485:GLU:HG3	1:A:486:LYS:CG	2.23	0.68
1:D:318:ASN:N	1:D:318:ASN:HD22	1.91	0.68
1:C:197:GLY:O	1:C:201:VAL:HG23	1.94	0.68
1:C:224:ASN:OD1	1:C:228:ARG:NH1	2.27	0.67
1:D:446:ARG:NH1	1:D:446:ARG:HB3	2.09	0.67
1:B:472:ARG:HG3	1:B:472:ARG:NH1	2.03	0.66
1:D:222:ARG:HD2	4:D:1487:CL:CL	2.33	0.66
1:D:321:ASN:HB3	8:D:2014:HOH:O	1.93	0.66
1:D:69:TYR:O	1:D:73:LEU:HG	1.95	0.66
1:D:306:LYS:H	1:D:306:LYS:HZ1	1.44	0.65
1:B:60:LYS:HE3	1:B:202:GLU:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:VAL:HG13	1:B:350:PHE:HD2	1.60	0.65
1:B:296:LEU:HD12	1:B:303:LEU:HD21	1.79	0.64
1:A:198:PHE:O	1:A:202:GLU:HG3	1.97	0.64
1:B:351:GLY:CA	1:B:352:ASN:CB	2.67	0.64
1:B:302:LYS:H	1:B:318:ASN:ND2	1.95	0.64
1:B:9:VAL:HB	1:B:33:VAL:HG22	1.79	0.64
1:B:129:LEU:HD23	1:B:299:VAL:CG2	2.28	0.64
1:B:302:LYS:HD3	1:B:310:GLN:NE2	2.13	0.63
1:D:227:LEU:HB2	1:D:235:ARG:HG2	1.81	0.63
1:D:314:PHE:O	1:D:315:SER:HB2	1.99	0.63
1:D:199:ILE:HB	7:D:1491:MPD:CM	2.29	0.63
1:D:287:ARG:HG3	7:D:1491:MPD:H32	1.81	0.63
1:D:104:LEU:HG	1:D:108:LYS:HE3	1.80	0.62
1:C:170:PRO:HG2	1:C:257:LYS:HB3	1.82	0.62
1:B:253:GLU:OE1	8:B:2023:HOH:O	2.16	0.62
1:C:348:THR:HG23	1:C:354:PRO:HA	1.80	0.62
1:A:59:PRO:HB3	1:A:99:LYS:HD3	1.82	0.62
1:B:60:LYS:HE3	1:B:202:GLU:CD	2.20	0.62
1:D:446:ARG:HB3	1:D:446:ARG:HH11	1.66	0.61
1:A:69:TYR:HA	1:A:72:HIS:HB2	1.83	0.60
1:D:396:PHE:CD1	1:D:396:PHE:N	2.68	0.60
1:B:44:PHE:CE1	1:B:126:TRP:HZ2	2.19	0.60
1:D:93:LYS:HE3	8:D:2024:HOH:O	2.01	0.60
1:B:448[B]:ASN:HD21	1:B:450:LYS:HZ3	1.47	0.60
1:D:243:THR:HA	1:D:247:ILE:O	2.01	0.60
1:A:132:LYS:HZ2	1:A:321:ASN:CB	2.13	0.60
1:D:352:ASN:ND2	1:D:352:ASN:C	2.55	0.60
1:D:286:GLY:HA2	7:D:1491:MPD:H13	1.84	0.60
1:C:440:ALA:HB3	1:D:440:ALA:HB3	1.83	0.60
1:B:17:LEU:HD12	3:B:1000:WP5:BRA	2.56	0.59
1:D:318:ASN:ND2	1:D:318:ASN:H	1.90	0.59
1:B:225:LEU:HB3	1:B:235:ARG:NH2	2.18	0.59
1:C:60:LYS:HE3	1:C:202:GLU:OE1	2.03	0.59
1:A:148:LYS:O	1:A:149:GLU:HG2	2.04	0.58
1:D:286:GLY:H	7:D:1491:MPD:C1	2.14	0.58
1:A:400:MET:HG3	1:A:401:HIS:N	2.18	0.58
1:B:130:GLU:HB2	1:B:136:VAL:HB	1.84	0.58
1:A:266:LYS:HE3	1:A:279:ASP:O	2.04	0.58
1:D:170:PRO:HG2	1:D:257:LYS:HB3	1.85	0.58
1:B:397:THR:OG1	1:B:410:LYS:NZ	2.37	0.57
1:D:227:LEU:HD12	1:D:238:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:ILE:HB	7:D:1491:MPD:HM1	1.86	0.57
1:B:167:PRO:O	1:B:172:ILE:HG12	2.03	0.57
1:D:13:GLY:HA3	2:D:998:FAD:H52A	1.85	0.57
1:C:358:ASP:OD2	1:C:446:ARG:NH2	2.37	0.57
1:B:253:GLU:OE1	1:B:253:GLU:HA	2.05	0.56
1:C:228:ARG:HE	1:C:235:ARG:HH22	1.52	0.56
1:B:351:GLY:HA2	1:B:352:ASN:CB	2.33	0.56
1:A:224:ASN:O	1:A:251:THR:HG21	2.05	0.56
1:C:69:TYR:HA	1:C:72:HIS:HB2	1.86	0.56
1:A:462:PRO:HG2	1:B:61:LYS:HG2	1.86	0.56
1:A:228:ARG:NH1	1:A:235:ARG:NH2	2.54	0.56
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.86	0.56
1:B:18:GLU:HG2	1:B:339:ILE:HG23	1.87	0.56
1:D:378:ILE:HG12	8:D:2045:HOH:O	2.05	0.56
1:C:155:HIS:ND1	1:C:323:TYR:OH	2.25	0.56
1:B:2:SER:C	1:B:3:LYS:HG2	2.26	0.56
1:B:104:LEU:O	1:B:108:LYS:HG3	2.04	0.55
1:C:198:PHE:HB2	1:C:366:VAL:HG13	1.89	0.55
1:C:131:SER:O	1:C:133:ASN:N	2.39	0.55
1:D:40:HIS:H	1:D:107:ASN:ND2	2.04	0.55
1:A:69:TYR:O	1:A:73:LEU:HG	2.07	0.55
1:D:434:ALA:HB3	1:D:435:PRO:HD3	1.88	0.55
1:C:40:HIS:H	1:C:107:ASN:ND2	2.05	0.55
1:D:341:GLU:OE2	1:D:359:HIS:HE1	1.89	0.55
1:B:250:MET:HE1	1:B:253:GLU:HG3	1.87	0.55
1:C:459:GLY:O	1:D:336:PRO:HG2	2.06	0.55
1:A:429:LEU:HD21	1:A:468:LEU:HD21	1.88	0.55
1:B:176:ILE:HB	1:B:180:GLU:HB2	1.89	0.54
1:C:4:ALA:HB2	1:C:152:GLN:HB2	1.89	0.54
1:A:331[B]:ARG:HB3	8:A:2050:HOH:O	2.06	0.54
1:D:341:GLU:OE2	1:D:359:HIS:CE1	2.60	0.54
1:A:129:LEU:HD23	1:A:299:VAL:HG21	1.88	0.54
1:A:75:GLU:OE2	1:A:409:LYS:NZ	2.37	0.54
1:A:148:LYS:C	1:A:149:GLU:HG2	2.28	0.54
1:B:95:LEU:HD22	1:B:210:TYR:CZ	2.42	0.54
1:A:413:ALA:HA	1:A:429:LEU:HD23	1.90	0.54
1:B:335:THR:HB	1:B:336:PRO:HD3	1.90	0.54
1:A:174:HIS:CE1	1:A:260:LEU:HG	2.43	0.53
1:A:286:GLY:CA	6:A:1491:MRD:O2	2.56	0.53
1:C:341:GLU:OE2	1:C:359:HIS:HE1	1.91	0.53
1:C:60:LYS:HE3	1:C:202:GLU:CD	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLY:HA2	1:A:327:ASP:HB2	1.91	0.53
1:A:132:LYS:NZ	1:A:320:PRO:O	2.40	0.53
1:C:241:GLN:OE1	1:C:370:PRO:HG3	2.08	0.53
1:D:8:VAL:HG22	1:D:32:ALA:HB3	1.91	0.53
1:C:265:SER:C	1:C:266:LYS:HD3	2.29	0.53
1:D:479:VAL:O	1:D:480:LYS:C	2.47	0.53
1:A:132:LYS:CE	1:A:320:PRO:O	2.57	0.52
2:D:998:FAD:O1A	2:D:998:FAD:H5'1	2.10	0.52
1:A:176:ILE:HB	1:A:180:GLU:HB2	1.91	0.52
1:A:302:LYS:H	1:A:318:ASN:ND2	2.06	0.52
1:C:110:TYR:CE2	3:C:1000:WP5:HAI	2.45	0.52
1:D:192:LEU:HA	1:D:218:THR:O	2.10	0.52
1:D:286:GLY:CA	7:D:1491:MPD:C1	2.88	0.52
1:D:318:ASN:ND2	1:D:318:ASN:N	2.54	0.52
1:C:110:TYR:CZ	3:C:1000:WP5:HAI	2.45	0.52
1:D:45:TYR:HB3	1:D:55:VAL:HG11	1.92	0.52
1:A:463:THR:O	1:A:466:GLU:HG2	2.09	0.52
1:B:257:LYS:HG3	8:B:2025:HOH:O	2.10	0.52
1:A:396:PHE:H	1:A:396:PHE:HD1	1.53	0.51
1:B:14:SER:HB2	2:B:998:FAD:O5'	2.10	0.51
1:D:52:CYS:HB2	1:D:335:THR:HG1	1.75	0.51
1:B:133:ASN:ND2	1:B:153:ALA:O	2.36	0.51
1:B:154:ASP:O	1:B:321:ASN:CG	2.48	0.51
1:B:18:GLU:CG	1:B:339:ILE:HG23	2.41	0.51
1:C:218:THR:HG23	1:C:248:GLU:HG2	1.92	0.51
1:B:331[B]:ARG:NH2	1:B:359:HIS:CD2	2.79	0.51
1:A:301:VAL:HA	1:A:318:ASN:HD21	1.75	0.51
1:D:302:LYS:H	1:D:318:ASN:HD21	1.58	0.51
1:A:118:GLU:OE1	1:A:118:GLU:HA	2.10	0.51
1:A:132:LYS:HE2	1:A:320:PRO:O	2.11	0.51
1:A:395:SER:HA	1:A:411:PHE:O	2.11	0.51
1:A:421:ASP:O	1:A:450:LYS:HD3	2.10	0.51
1:B:348:THR:HA	1:B:354:PRO:HA	1.93	0.51
1:B:253:GLU:OE1	1:B:272:SER:HB3	2.11	0.50
1:C:295:GLN:NE2	1:C:295:GLN:CA	2.72	0.50
1:C:60:LYS:HD2	1:C:61:LYS:N	2.26	0.50
1:C:447:LEU:HD11	1:D:449:ALA:HB2	1.93	0.50
1:D:126:TRP:CD1	1:D:140:THR:HA	2.46	0.50
1:B:408:TYR:CE2	1:B:409:LYS:HG3	2.46	0.50
1:C:302:LYS:HG2	1:C:310:GLN:NE2	2.27	0.50
1:A:21:TRP:NE1	3:A:1000:WP5:HAW3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ARG:HG3	6:A:1491:MRD:H4	1.94	0.50
1:D:171:GLY:HA3	1:D:258:VAL:O	2.12	0.50
1:B:463:THR:O	1:B:466:GLU:HG2	2.12	0.50
1:D:360:THR:HB	7:D:1492:MPD:HM1	1.93	0.50
1:D:164:PRO:HB3	7:D:1491:MPD:C5	2.30	0.50
1:D:302:LYS:H	1:D:318:ASN:ND2	2.09	0.50
1:D:352:ASN:C	1:D:352:ASN:HD22	2.15	0.49
1:B:197:GLY:O	1:B:201:VAL:HG23	2.13	0.49
1:C:224:ASN:N	1:C:224:ASN:OD1	2.31	0.49
1:C:52:CYS:HB2	1:C:335:THR:OG1	2.12	0.49
1:D:190:ARG:HB2	1:D:278:VAL:HA	1.94	0.49
1:C:126:TRP:CD1	1:C:140:THR:HA	2.48	0.49
1:C:81:TRP:NE1	1:D:69:TYR:HB2	2.25	0.49
1:D:189:ARG:HB3	1:D:279:ASP:OD2	2.12	0.49
1:D:92:TRP:O	1:D:93:LYS:C	2.51	0.49
1:C:109:SER:O	1:C:113:MET:HG3	2.13	0.49
1:D:390:ALA:HB3	1:D:417:THR:OG1	2.13	0.49
1:B:44:PHE:CZ	1:B:126:TRP:HZ2	2.31	0.49
1:C:295:GLN:HA	1:C:295:GLN:HE21	1.76	0.49
1:C:40:HIS:H	1:C:107:ASN:HD21	1.60	0.49
1:D:352:ASN:HD22	1:D:353:LYS:N	2.11	0.49
1:C:392:TYR:O	1:C:414:LYS:HA	2.12	0.49
1:B:477:TYR:O	1:B:483:LYS:HA	2.12	0.49
1:A:349:VAL:HG12	1:A:350:PHE:CD2	2.48	0.48
1:B:63:MET:HA	1:B:95:LEU:HD11	1.96	0.48
1:D:261:ASN:OD1	1:D:267:HIS:HB2	2.13	0.48
1:D:8:VAL:CG2	1:D:153:ALA:HB2	2.44	0.48
1:B:263:ASP:C	1:B:263:ASP:OD1	2.52	0.48
1:D:221:TYR:CE2	1:D:223:ASN:HB2	2.48	0.48
1:D:485:GLU:O	1:D:485:GLU:CG	2.46	0.48
1:D:321:ASN:HB2	8:D:2014:HOH:O	2.05	0.48
1:A:232:GLU:OE1	8:A:2026:HOH:O	2.20	0.48
1:B:341:GLU:OE2	1:B:359:HIS:HE1	1.96	0.48
1:A:186:GLU:HB2	1:A:187:PRO:HD2	1.96	0.48
1:C:345:LEU:HA	8:C:2020:HOH:O	2.14	0.48
1:B:461:HIS:HA	1:B:462:PRO:HA	1.71	0.47
1:A:439:GLN:OE1	1:B:466:GLU:HA	2.14	0.47
1:A:63:MET:HG2	1:A:95:LEU:HD21	1.97	0.47
1:B:104:LEU:O	1:B:107:ASN:HB2	2.15	0.47
1:A:132:LYS:HZ1	1:A:321:ASN:CB	2.22	0.47
1:B:346:VAL:HG13	1:B:350:PHE:CD2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:GLU:HB2	1:D:136:VAL:HG23	1.95	0.47
1:D:399:LEU:HD12	1:D:402:ASN:HB2	1.95	0.47
1:D:45:TYR:CD2	1:D:45:TYR:N	2.81	0.47
1:B:220:CYS:HA	1:B:250:MET:O	2.14	0.47
1:D:129:LEU:HD11	1:D:156:ILE:HG21	1.97	0.47
1:A:460:VAL:HG13	1:B:364:SER:HA	1.96	0.47
1:D:21:TRP:CD1	3:D:1000:WP5:HAW3	2.50	0.47
1:A:306:LYS:H	1:A:306:LYS:CD	2.27	0.47
1:B:142:ASP:C	1:B:144:LYS:H	2.18	0.46
1:D:479:VAL:HG22	1:D:480:LYS:H	1.80	0.46
1:B:415:ILE:HG13	1:B:471:MET:CE	2.45	0.46
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.49	0.46
1:D:199:ILE:HB	7:D:1491:MPD:HM2	1.98	0.46
1:D:377:LEU:HG	7:D:1492:MPD:H4	1.97	0.46
1:B:154:ASP:O	1:B:321:ASN:ND2	2.48	0.46
1:C:137:VAL:O	1:C:148:LYS:HB2	2.15	0.46
1:C:460:VAL:HG13	1:D:364:SER:HA	1.98	0.46
1:D:306:LYS:NZ	1:D:306:LYS:H	2.13	0.46
1:A:286:GLY:N	6:A:1491:MRD:O2	2.49	0.46
1:C:131:SER:O	1:C:134:VAL:N	2.40	0.46
1:C:341:GLU:OE2	1:C:359:HIS:CE1	2.69	0.46
1:D:212:PRO:CB	1:D:213:PRO:HD2	2.46	0.45
1:B:411:PHE:CD1	1:B:431:GLY:HA3	2.51	0.45
1:B:61:LYS:HE3	1:B:367:PHE:CE1	2.51	0.45
1:A:441:VAL:O	1:A:444:CYS:HB2	2.17	0.45
1:D:461:HIS:HA	1:D:462:PRO:HA	1.61	0.45
1:B:157:LEU:HD12	1:B:158:LEU:N	2.31	0.45
1:C:142:ASP:HA	1:C:143:PRO:HD3	1.84	0.45
1:C:417:THR:HG21	1:C:451:ILE:HB	1.99	0.45
1:D:202:GLU:O	1:D:206:ILE:HG13	2.17	0.45
1:D:387:GLU:HG3	1:D:480:LYS:HD3	1.99	0.45
1:A:366:VAL:HB	1:A:372:ILE:HB	1.99	0.45
1:A:461:HIS:HA	1:A:462:PRO:HA	1.81	0.45
1:A:69:TYR:CD1	1:B:76:SER:HB3	2.51	0.45
1:C:129:LEU:HD11	1:C:156:ILE:HG21	1.98	0.45
1:D:320:PRO:O	1:D:321:ASN:HB2	2.17	0.45
1:A:173:GLU:OE1	1:A:173:GLU:N	2.44	0.44
1:B:351:GLY:HA2	1:B:352:ASN:ND2	2.32	0.44
1:C:227:LEU:HB2	1:C:235:ARG:HG2	1.99	0.44
1:C:461:HIS:HA	1:C:462:PRO:HA	1.76	0.44
1:B:34:VAL:HA	1:B:123:PHE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:HD22	1:B:247:ILE:HD12	2.00	0.44
1:B:479:VAL:C	1:B:481:GLY:H	2.20	0.44
1:D:283:MET:O	7:D:1491:MPD:H52	2.18	0.44
1:D:301:VAL:HA	1:D:318:ASN:HD21	1.82	0.44
1:C:370:PRO:HG3	8:C:2015:HOH:O	2.15	0.44
1:D:348:THR:HA	1:D:354:PRO:HA	1.99	0.44
1:A:451:ILE:O	1:A:454:PHE:HB2	2.17	0.44
1:B:392:TYR:O	1:B:414:LYS:HA	2.17	0.44
1:D:140:THR:HB	8:D:2015:HOH:O	2.18	0.44
1:D:360:THR:HB	7:D:1492:MPD:O4	2.17	0.44
1:A:13:GLY:HA2	1:A:50:GLY:HA3	1.99	0.44
1:A:436:GLU:HB3	1:B:437:ILE:HG12	1.99	0.44
1:B:270:PHE:HB3	8:B:2023:HOH:O	2.17	0.44
1:D:52:CYS:HB2	1:D:335:THR:OG1	2.17	0.44
1:B:378:ILE:HD12	1:B:380:GLU:OE1	2.17	0.44
1:D:387:GLU:O	1:D:479:VAL:HA	2.18	0.44
1:D:40:HIS:H	1:D:107:ASN:HD21	1.66	0.43
1:A:287:ARG:CG	6:A:1491:MRD:H1C2	2.47	0.43
6:A:1491:MRD:HMC1	8:A:2041:HOH:O	2.18	0.43
1:A:396:PHE:CD1	1:A:396:PHE:N	2.72	0.43
1:C:399:LEU:O	1:C:400:MET:C	2.54	0.43
1:D:241:GLN:NE2	1:D:410:LYS:H	2.16	0.43
1:D:41:GLY:O	1:D:45:TYR:N	2.45	0.43
1:C:130:GLU:OE1	1:C:134:VAL:HG11	2.17	0.43
1:C:38:THR:O	1:C:48:LEU:HB3	2.18	0.43
1:D:480:LYS:HA	1:D:480:LYS:HD2	1.88	0.43
1:A:353:LYS:HA	1:A:354:PRO:HD2	1.84	0.43
1:B:242:LEU:CD2	1:B:247:ILE:HD12	2.48	0.43
1:A:453:ASP:OD2	1:B:447:LEU:HD21	2.17	0.43
1:C:314:PHE:O	1:C:315:SER:HB2	2.18	0.43
1:C:331[B]:ARG:NH2	1:C:359:HIS:CD2	2.87	0.43
1:D:44:PHE:O	1:D:46:ALA:N	2.50	0.43
2:D:998:FAD:PA	2:D:998:FAD:H5'1	2.58	0.43
1:B:479:VAL:C	1:B:481:GLY:N	2.72	0.43
1:D:190:ARG:HD2	1:D:277:ASP:O	2.19	0.43
1:A:190:ARG:HB3	1:A:278:VAL:HG12	2.00	0.43
1:B:438:ILE:O	1:B:441:VAL:HB	2.18	0.43
1:C:449:ALA:HB1	1:C:454:PHE:HE2	1.83	0.43
1:C:4:ALA:CB	1:C:152:GLN:HB2	2.49	0.43
1:A:320:PRO:O	1:A:321:ASN:HB2	2.18	0.43
1:B:268:VAL:O	1:B:275:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:ILE:O	1:D:328:ILE:HG12	2.18	0.43
1:D:63:MET:HG2	1:D:95:LEU:HD21	2.00	0.43
1:B:366:VAL:HB	1:B:372:ILE:HB	2.01	0.43
1:B:44:PHE:CE1	1:B:126:TRP:CZ2	3.04	0.43
1:D:249:ILE:HG22	1:D:251:THR:HG23	2.00	0.43
1:B:265:SER:HB2	1:B:278:VAL:O	2.19	0.43
1:A:408:TYR:CE2	1:A:409:LYS:HG3	2.54	0.42
1:D:188:PRO:HD2	8:D:2026:HOH:O	2.18	0.42
1:A:171:GLY:HA3	1:A:258:VAL:O	2.19	0.42
1:D:9:VAL:HG22	1:D:157:LEU:HB3	2.00	0.42
1:A:35:ASP:OD1	1:A:36:VAL:N	2.51	0.42
1:A:438:ILE:HA	1:A:438:ILE:HD12	1.88	0.42
1:C:15:GLY:HA3	1:C:325:ILE:HD13	2.00	0.42
1:D:361:ARG:HG3	7:D:1492:MPD:H53	2.01	0.42
1:B:415:ILE:HG13	1:B:471:MET:HE1	2.02	0.42
1:A:285:ILE:N	6:A:1491:MRD:H5C3	2.34	0.42
1:A:320:PRO:C	1:A:322:ILE:H	2.23	0.42
1:B:18:GLU:OE1	3:B:1000:WP5:NAT	2.52	0.42
1:C:69:TYR:CD1	1:D:76:SER:HB3	2.55	0.42
1:A:91:ASN:HB3	1:B:80:GLY:O	2.19	0.42
1:C:60:LYS:CD	1:C:60:LYS:C	2.88	0.42
1:A:27:TYR:HE2	1:A:346:VAL:HG12	1.83	0.42
1:B:21:TRP:CD1	3:B:1000:WP5:HAW3	2.55	0.42
1:C:474:PRO:HG2	1:C:477:TYR:OH	2.20	0.42
1:D:199:ILE:HD12	7:D:1491:MPD:CM	2.49	0.42
1:D:337:VAL:O	1:D:341:GLU:HB2	2.20	0.42
1:A:62:LEU:HA	1:A:62:LEU:HD23	1.93	0.42
1:D:408:TYR:CE2	1:D:409:LYS:HG3	2.54	0.42
1:A:437:ILE:HG12	1:A:465:ALA:HB2	2.02	0.42
1:B:479:VAL:O	1:B:481:GLY:N	2.53	0.42
1:C:176:ILE:HB	1:C:180:GLU:HB2	2.02	0.42
1:C:379:GLU:OE1	1:C:414:LYS:NZ	2.50	0.42
1:D:237:GLU:OE1	1:D:240:LYS:NZ	2.53	0.42
1:D:190:ARG:HA	1:D:216:LYS:O	2.20	0.41
1:A:155:HIS:HB3	1:A:323:TYR:HE2	1.84	0.41
1:A:485:GLU:C	1:A:486:LYS:HG2	2.40	0.41
1:B:22:ASN:O	1:B:26:LEU:HB2	2.20	0.41
1:B:353:LYS:HA	1:B:354:PRO:HD2	1.83	0.41
7:D:1491:MPD:HM1	7:D:1491:MPD:H4	1.89	0.41
1:D:352:ASN:O	1:D:354:PRO:HD2	2.20	0.41
1:B:63:MET:HB2	1:B:206:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:TYR:CZ	1:C:474:PRO:HG3	2.56	0.41
1:D:361:ARG:N	7:D:1492:MPD:O2	2.45	0.41
1:B:110:TYR:CE2	3:B:1000:WP5:HAI	2.56	0.41
1:C:449:ALA:HB1	1:C:454:PHE:CE2	2.54	0.41
1:A:228:ARG:HG2	1:A:228:ARG:HH11	1.85	0.41
1:A:249:ILE:HG22	1:A:249:ILE:O	2.20	0.41
1:C:331[B]:ARG:HH21	1:C:359:HIS:CD2	2.38	0.41
1:A:212:PRO:CB	1:A:213:PRO:HD2	2.51	0.41
1:B:473:THR:HA	1:B:474:PRO:HD3	1.91	0.41
1:B:60:LYS:HD2	1:B:61:LYS:N	2.35	0.41
1:D:51:THR:O	1:D:52:CYS:C	2.59	0.41
1:A:228:ARG:CG	1:A:228:ARG:HH11	2.33	0.41
1:A:398:PRO:HD3	1:A:411:PHE:H	1.86	0.41
1:C:63:MET:HG2	1:C:95:LEU:HD21	2.03	0.41
1:D:393:MET:HG3	1:D:414:LYS:CG	2.51	0.41
1:C:39:SER:HA	1:C:107:ASN:ND2	2.36	0.41
1:A:447:LEU:HD23	1:A:447:LEU:HA	1.88	0.40
1:B:274[B]:LYS:HE2	1:B:274[B]:LYS:HB2	1.47	0.40
1:C:64:VAL:HG23	1:C:206:ILE:HD11	2.03	0.40
1:C:480:LYS:HA	1:C:480:LYS:HD2	1.71	0.40
1:D:475:SER:O	1:D:476:TYR:HB3	2.20	0.40
1:A:478:TYR:HA	1:A:482:GLU:O	2.21	0.40
1:C:396:PHE:H	1:C:396:PHE:HD1	1.66	0.40
1:A:92:TRP:O	1:A:96:ILE:HG12	2.22	0.40
1:B:455:TYR:HB2	1:B:472:ARG:NH1	2.37	0.40
1:A:90:ALA:HB2	1:B:81:TRP:CH2	2.57	0.40
1:C:40:HIS:N	1:C:107:ASN:ND2	2.70	0.40
1:C:292:ASN:HB2	8:C:2019:HOH:O	2.21	0.40
1:D:7:LEU:HB3	1:D:31:VAL:HG22	2.03	0.40
1:D:461:HIS:HD1	1:D:466:GLU:CD	2.24	0.40
1:A:8:VAL:HG22	1:A:32:ALA:HB3	2.03	0.40
1:B:95:LEU:HD22	1:B:210:TYR:CE2	2.57	0.40
1:B:9:VAL:HG22	1:B:157:LEU:HB3	2.02	0.40
1:C:295:GLN:CA	1:C:295:GLN:HE21	2.34	0.40
1:A:411:PHE:CD1	1:A:431:GLY:HA3	2.57	0.40
1:A:75:GLU:HA	8:A:2061:HOH:O	2.21	0.40
1:B:321:ASN:HD22	1:B:321:ASN:HA	1.72	0.40
1:D:400:MET:HG3	1:D:401:HIS:N	2.36	0.40

There are no symmetry-related clashes.

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	489/495 (99%)	456 (93%)	31 (6%)	2 (0%)	36	70
1	B	488/495 (99%)	440 (90%)	41 (8%)	7 (1%)	12	38
1	C	485/495 (98%)	446 (92%)	32 (7%)	7 (1%)	12	38
1	D	487/495 (98%)	450 (92%)	33 (7%)	4 (1%)	21	53
All	All	1949/1980 (98%)	1792 (92%)	137 (7%)	20 (1%)	17	48

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	LYS
1	C	132	LYS
1	C	133	ASN
1	D	213	PRO
1	C	298	ASN
1	C	352	ASN
1	D	480	LYS
1	B	271	GLU
1	B	320	PRO
1	B	352	ASN
1	B	480	LYS
1	B	45	TYR
1	B	252	ASN
1	D	331	ARG
1	A	352	ASN
1	B	476	TYR
1	C	45	TYR
1	C	465	ALA
1	D	45	TYR
1	C	213	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	404/407 (99%)	382 (95%)	22 (5%)	24	56
1	B	403/407 (99%)	369 (92%)	34 (8%)	12	34
1	C	400/407 (98%)	361 (90%)	39 (10%)	9	26
1	D	402/407 (99%)	375 (93%)	27 (7%)	18	46
All	All	1609/1628 (99%)	1487 (92%)	122 (8%)	15	39

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	57	CYS
1	A	60	LYS
1	A	86	SER
1	A	99	LYS
1	A	132	LYS
1	A	191	VAL
1	A	222	ARG
1	A	228	ARG
1	A	238	VAL
1	A	251	THR
1	A	266	LYS
1	A	306	LYS
1	A	331[A]	ARG
1	A	331[B]	ARG
1	A	393	MET
1	A	400	MET
1	A	446	ARG
1	A	455[A]	TYR
1	A	455[B]	TYR
1	A	455[C]	TYR
1	A	486	LYS
1	B	3	LYS
1	B	57	CYS

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Mol	Chain	Res	Type
1	B	60	LYS
1	B	99	LYS
1	B	111	GLU
1	B	129	LEU
1	B	136	VAL
1	B	150	ARG
1	B	152	GLN
1	B	154	ASP
1	B	160	THR
1	B	162	SER
1	B	165	GLN
1	B	172	ILE
1	B	178	SER
1	B	238	VAL
1	B	260	LEU
1	B	291	THR
1	B	292	ASN
1	B	293	ASP
1	B	306	LYS
1	B	320	PRO
1	B	321	ASN
1	B	331[A]	ARG
1	B	331[B]	ARG
1	B	356	LYS
1	B	400	MET
1	B	407	LYS
1	B	420	SER
1	B	472	ARG
1	B	473	THR
1	B	475	SER
1	B	485	GLU
1	B	486	LYS
1	C	2	SER
1	C	5	PHE
1	C	35	ASP
1	C	39	SER
1	C	57	CYS
1	C	60	LYS
1	C	94	LYS
1	C	99	LYS
1	C	108	LYS
1	C	120	LEU

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Mol	Chain	Res	Type
1	C	128	SER
1	C	129	LEU
1	C	132	LYS
1	C	136	VAL
1	C	139	GLU
1	C	224	ASN
1	C	248	GLU
1	C	249	ILE
1	C	260	LEU
1	C	262	THR
1	C	266	LYS
1	C	288	ILE
1	C	289	PRO
1	C	295	GLN
1	C	299	VAL
1	C	304	THR
1	C	306	LYS
1	C	323	TYR
1	C	331[A]	ARG
1	C	331[B]	ARG
1	C	388	LYS
1	C	399	LEU
1	C	400	MET
1	C	407	LYS
1	C	448	ASN
1	C	460	VAL
1	C	480	LYS
1	C	485	GLU
1	C	486	LYS
1	D	2	SER
1	D	57	CYS
1	D	60	LYS
1	D	99	LYS
1	D	129	LEU
1	D	138	ARG
1	D	149	GLU
1	D	198	PHE
1	D	213	PRO
1	D	228	ARG
1	D	237	GLU
1	D	242	LEU
1	D	266	LYS

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Mol	Chain	Res	Type
1	D	274	LYS
1	D	288	ILE
1	D	306	LYS
1	D	313	GLU
1	D	318	ASN
1	D	321	ASN
1	D	331	ARG
1	D	335	THR
1	D	352	ASN
1	D	353	LYS
1	D	396	PHE
1	D	406	SER
1	D	446	ARG
1	D	486	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	ASN
1	A	318	ASN
1	A	321	ASN
1	A	359	HIS
1	A	402	ASN
1	B	107	ASN
1	B	252	ASN
1	B	310	GLN
1	B	318	ASN
1	B	321	ASN
1	B	352	ASN
1	B	359	HIS
1	C	107	ASN
1	C	295	GLN
1	C	310	GLN
1	C	359	HIS
1	C	419	HIS
1	D	107	ASN
1	D	152	GLN
1	D	318	ASN
1	D	321	ASN
1	D	352	ASN
1	D	359	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 for Mogul analysis.

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	WP5	A	1000	-	25,25,25	2.47	6 (24%)	30,35,35	1.66	4 (13%)
6	MRD	A	1491	-	7,7,7	0.48	0	9,10,10	2.01	2 (22%)
6	MRD	A	1492	-	7,7,7	0.42	0	9,10,10	1.35	2 (22%)
2	FAD	A	998	-	51,58,58	1.41	9 (17%)	57,89,89	2.10	10 (17%)
3	WP5	B	1000	-	25,25,25	1.87	4 (16%)	30,35,35	1.80	8 (26%)
2	FAD	B	998	-	51,58,58	1.48	11 (21%)	57,89,89	2.00	6 (10%)
3	WP5	C	1000	-	25,25,25	2.51	6 (24%)	30,35,35	1.92	5 (16%)
2	FAD	C	998	-	51,58,58	1.33	6 (11%)	57,89,89	2.37	9 (15%)
3	WP5	D	1000	-	25,25,25	2.31	5 (20%)	30,35,35	1.57	3 (10%)
7	MPD	D	1491	-	7,7,7	0.50	0	9,10,10	1.35	1 (11%)
7	MPD	D	1492	-	7,7,7	0.44	0	9,10,10	1.22	1 (11%)
2	FAD	D	998	-	51,58,58	1.34	5 (9%)	57,89,89	2.15	11 (19%)

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	WP5	A	1000	-	-	0/10/26/26	0/3/3/3
6	MRD	A	1491	-	-	0/5/5/5	0/0/0/0
6	MRD	A	1492	-	-	0/5/5/5	0/0/0/0
2	FAD	A	998	-	-	0/28/50/50	0/6/6/6
3	WP5	B	1000	-	-	0/10/26/26	0/3/3/3
2	FAD	B	998	-	-	0/28/50/50	0/6/6/6
3	WP5	C	1000	-	-	0/10/26/26	0/3/3/3
2	FAD	C	998	-	-	0/28/50/50	0/6/6/6
3	WP5	D	1000	-	-	0/10/26/26	0/3/3/3
7	MPD	D	1491	-	-	0/5/5/5	0/0/0/0
7	MPD	D	1492	-	-	0/5/5/5	0/0/0/0
2	FAD	D	998	-	-	0/28/50/50	0/6/6/6

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	998	FAD	C6-C5X	-2.42	1.38	1.41
2	B	998	FAD	C4-C4X	-2.27	1.37	1.41
2	A	998	FAD	O4B-C4B	-2.18	1.40	1.45
2	B	998	FAD	O4B-C4B	-2.10	1.40	1.45
2	A	998	FAD	C9-C8	2.11	1.43	1.37
2	B	998	FAD	C9A-N10	2.11	1.41	1.38
2	C	998	FAD	C2A-N1A	2.12	1.37	1.33
2	B	998	FAD	C5X-N5	2.17	1.38	1.35
2	B	998	FAD	C1'-N10	2.20	1.50	1.48
2	D	998	FAD	C1'-N10	2.24	1.50	1.48
2	A	998	FAD	C5'-C4'	2.29	1.55	1.51
3	D	1000	WP5	CAW-CAU	2.40	1.53	1.49
2	C	998	FAD	C5X-N5	2.44	1.39	1.35
2	A	998	FAD	C2A-N1A	2.60	1.38	1.33
3	B	1000	WP5	CAW-CAU	2.61	1.53	1.49
2	B	998	FAD	C2A-N1A	2.63	1.38	1.33
2	D	998	FAD	C4-N3	2.77	1.38	1.33
2	B	998	FAD	C4-N3	2.77	1.38	1.33
2	C	998	FAD	C2A-N3A	2.78	1.36	1.32
3	B	1000	WP5	CA-N	2.85	1.48	1.45
2	C	998	FAD	C4-N3	2.92	1.38	1.33
2	A	998	FAD	C4-N3	2.97	1.38	1.33
3	C	1000	WP5	CAJ-CAK	3.11	1.55	1.51
2	D	998	FAD	C2A-N3A	3.14	1.37	1.32
3	A	1000	WP5	CAW-CAU	3.15	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1000	WP5	CAU-N	3.18	1.42	1.35
3	D	1000	WP5	CAK-N	3.23	1.50	1.48
2	D	998	FAD	C4X-N5	3.31	1.38	1.33
3	C	1000	WP5	CAW-CAU	3.31	1.54	1.49
3	A	1000	WP5	CAE-CAK	3.33	1.56	1.52
2	B	998	FAD	C10-N1	3.36	1.37	1.33
2	A	998	FAD	C10-N1	3.36	1.37	1.33
2	A	998	FAD	C4X-N5	3.39	1.38	1.33
2	A	998	FAD	C2A-N3A	3.42	1.37	1.32
2	C	998	FAD	C4X-N5	3.52	1.38	1.33
3	B	1000	WP5	CAU-N	3.53	1.43	1.35
2	B	998	FAD	C4X-N5	3.71	1.38	1.33
2	D	998	FAD	C10-N1	3.76	1.38	1.33
2	A	998	FAD	C5X-N5	3.86	1.41	1.35
3	D	1000	WP5	CAU-N	4.28	1.44	1.35
3	A	1000	WP5	CAU-N	4.33	1.44	1.35
3	A	1000	WP5	CAK-N	4.48	1.50	1.48
2	B	998	FAD	C2A-N3A	4.55	1.39	1.32
2	C	998	FAD	C10-N1	4.67	1.39	1.33
3	C	1000	WP5	CAE-CAK	4.76	1.57	1.52
3	A	1000	WP5	CA-N	4.84	1.50	1.45
3	D	1000	WP5	CA-N	4.87	1.50	1.45
3	C	1000	WP5	CA-N	5.00	1.50	1.45
3	B	1000	WP5	CAU-NAT	6.61	1.39	1.29
3	A	1000	WP5	CAU-NAT	7.32	1.40	1.29
3	C	1000	WP5	CAU-NAT	7.88	1.41	1.29
3	D	1000	WP5	CAU-NAT	8.07	1.41	1.29

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	998	FAD	N3A-C2A-N1A	-13.54	117.27	128.86
2	B	998	FAD	N3A-C2A-N1A	-10.89	119.55	128.86
2	A	998	FAD	N3A-C2A-N1A	-9.71	120.55	128.86
2	D	998	FAD	N3A-C2A-N1A	-8.85	121.29	128.86
2	D	998	FAD	C4B-O4B-C1B	-6.49	103.06	109.83
6	A	1491	MRD	CM-C2-C1	-4.52	100.84	110.51
3	D	1000	WP5	CAE-CAK-N	-3.80	105.92	111.60
3	B	1000	WP5	CAW-CAU-NAT	-3.73	115.40	119.56
3	D	1000	WP5	CAP-OAO-C	-3.55	104.06	116.14
2	A	998	FAD	C4X-C4-N3	-2.91	119.33	123.47
3	C	1000	WP5	CAE-CAK-N	-2.82	107.38	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1000	WP5	CAE-CAK-CAJ	-2.81	107.85	112.79
2	B	998	FAD	C4A-C5A-N7A	-2.79	106.71	109.41
2	C	998	FAD	C9A-C5X-N5	-2.62	118.61	122.32
7	D	1491	MPD	CM-C2-C1	-2.61	104.93	110.51
2	D	998	FAD	C4X-C4-N3	-2.57	119.81	123.47
7	D	1492	MPD	O2-C2-C1	-2.55	99.62	108.03
2	C	998	FAD	O2'-C2'-C1'	-2.54	103.33	109.61
3	B	1000	WP5	CAE-CAK-N	-2.54	107.81	111.60
3	B	1000	WP5	CAJ-CAS-NAT	-2.52	119.86	122.04
2	A	998	FAD	C10-C4X-N5	-2.51	117.71	120.59
2	D	998	FAD	N6A-C6A-N1A	-2.46	113.47	118.57
2	B	998	FAD	P-O3P-PA	-2.41	124.53	132.63
3	A	1000	WP5	CAE-CAK-CAJ	-2.29	108.75	112.79
6	A	1492	MRD	O2-C2-CM	-2.29	100.47	108.03
2	B	998	FAD	O3B-C3B-C4B	-2.25	104.53	111.06
3	A	1000	WP5	CAW-CAU-NAT	-2.25	117.05	119.56
3	C	1000	WP5	CAQ-CAH-CAI	-2.12	118.34	121.45
2	D	998	FAD	O2'-C2'-C3'	-2.10	103.90	109.10
6	A	1492	MRD	O2-C2-C1	-2.05	101.25	108.03
3	C	1000	WP5	CAJ-CAS-NAT	-2.04	120.28	122.04
2	C	998	FAD	O3B-C3B-C4B	-2.02	105.21	111.06
3	B	1000	WP5	CAJ-CAK-N	2.02	113.62	110.56
2	D	998	FAD	O5B-C5B-C4B	2.09	116.28	109.00
2	A	998	FAD	C2B-C3B-C4B	2.11	106.66	102.62
2	A	998	FAD	C7-C6-C5X	2.14	124.37	121.17
2	A	998	FAD	C6-C5X-N5	2.15	121.42	118.95
2	D	998	FAD	O4B-C4B-C5B	2.16	116.56	109.39
3	B	1000	WP5	CAD-CAE-CAF	2.16	121.01	118.30
6	A	1491	MRD	C1-C2-C3	2.40	121.27	109.94
2	B	998	FAD	C4X-N5-C5X	2.44	119.32	116.76
2	D	998	FAD	C4X-N5-C5X	2.47	119.35	116.76
2	C	998	FAD	C2A-N1A-C6A	2.54	123.06	118.75
3	A	1000	WP5	CAS-NAT-CAU	2.64	121.14	118.26
2	D	998	FAD	C5X-C9A-N10	2.87	119.91	117.71
2	A	998	FAD	C1'-N10-C9A	2.88	120.87	118.31
2	C	998	FAD	C5X-C9A-N10	3.07	120.06	117.71
2	C	998	FAD	C1'-N10-C9A	3.25	121.20	118.31
2	C	998	FAD	C4X-N5-C5X	3.62	120.55	116.76
3	B	1000	WP5	CAS-NAT-CAU	3.62	122.20	118.26
2	D	998	FAD	C1'-N10-C9A	3.91	121.79	118.31
2	A	998	FAD	C4-C4X-N5	3.96	123.15	118.70
3	C	1000	WP5	CAS-NAT-CAU	3.97	122.59	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	998	FAD	C4X-N5-C5X	4.25	121.21	116.76
3	D	1000	WP5	OAO-C-CA	4.48	118.11	110.25
3	B	1000	WP5	OAO-C-CA	4.71	118.50	110.25
2	C	998	FAD	C4-N3-C2	5.72	120.02	115.14
3	A	1000	WP5	OAO-C-CA	5.75	120.34	110.25
2	B	998	FAD	C4-N3-C2	5.84	120.12	115.14
2	A	998	FAD	C4-N3-C2	6.79	120.92	115.14
2	D	998	FAD	C4-N3-C2	6.98	121.09	115.14
3	C	1000	WP5	OAO-C-CA	7.04	122.61	110.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	WP5	2	0
6	A	1491	MRD	9	0
3	B	1000	WP5	4	0
2	B	998	FAD	2	0
3	C	1000	WP5	2	0
3	D	1000	WP5	1	0
7	D	1491	MPD	20	0
7	D	1492	MPD	6	0
2	D	998	FAD	3	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 [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, 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	488/495 (98%)	-0.90	0 100 100	2, 11, 25, 38	0
1	B	485/495 (97%)	-0.79	0 100 100	4, 16, 35, 41	0
1	C	485/495 (97%)	-0.79	1 (0%) 94 94	4, 16, 36, 49	0
1	D	488/495 (98%)	-0.87	0 100 100	3, 13, 27, 49	0
All	All	1946/1980 (98%)	-0.84	1 (0%) 95 95	2, 14, 34, 49	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	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. 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	B-factors(Å ²)	Q<0.9
5	NA	D	1490	1/1	0.89	0.16	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MPD	D	1491	8/8	0.92	0.30	33,36,40,41	0
7	MPD	D	1492	8/8	0.93	0.28	40,41,42,43	0
6	MRD	A	1492	8/8	0.94	0.18	19,20,21,22	0
5	NA	B	1490	1/1	0.95	0.06	20,20,20,20	0
5	NA	D	1489	1/1	0.95	0.10	30,30,30,30	0
5	NA	A	1490	1/1	0.96	0.14	16,16,16,16	0
6	MRD	A	1491	8/8	0.96	0.19	11,15,22,22	0
5	NA	C	1489	1/1	0.96	0.14	25,25,25,25	0
2	FAD	B	998	53/53	0.97	0.12	8,11,25,26	0
3	WP5	B	1000	23/23	0.98	0.11	22,24,27,31	0
4	CL	C	1488	1/1	0.98	0.05	21,21,21,21	0
3	WP5	C	1000	23/23	0.98	0.13	31,34,37,37	0
3	WP5	A	1000	23/23	0.98	0.11	14,20,23,25	0
5	NA	B	1489	1/1	0.98	0.11	11,11,11,11	0
2	FAD	C	998	53/53	0.98	0.10	2,12,22,25	0
3	WP5	D	1000	23/23	0.98	0.11	19,21,25,27	0
4	CL	A	1488	1/1	0.99	0.05	5,5,5,5	0
4	CL	B	1488	1/1	0.99	0.06	8,8,8,8	0
4	CL	D	1487	1/1	0.99	0.09	5,5,5,5	0
2	FAD	D	998	53/53	0.99	0.10	4,8,14,15	0
4	CL	C	1487	1/1	0.99	0.06	7,7,7,7	0
4	CL	B	1487	1/1	0.99	0.07	9,9,9,9	0
4	CL	A	1489	1/1	0.99	0.05	7,7,7,7	0
2	FAD	A	998	53/53	0.99	0.10	2,6,10,13	0
4	CL	D	1488	1/1	1.00	0.03	13,13,13,13	0

6.5 Other polymers

There are no such residues in this entry.