



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:47 PM GMT

PDB ID : 2ZZC
Title : Crystal structure of NADP(H):human thioredoxin reductase I
Authors : Lo, Y.C.; Ko, T.P.; Wang, A.H.J.
Deposited on : 2009-02-09
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

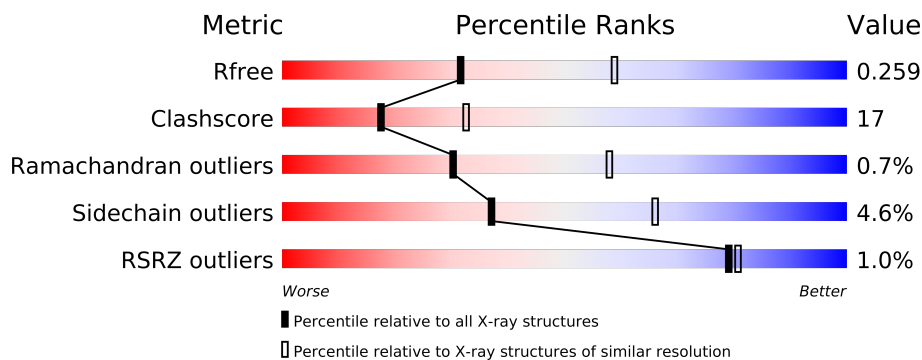
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	513	
1	B	513	
1	C	513	
1	D	513	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16283 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Thioredoxin reductase 1, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3750	2384	640	707	19			
1	B	484	Total	C	N	O	S	0	0	0
			3741	2379	638	705	19			
1	C	485	Total	C	N	O	S	0	0	0
			3750	2384	640	707	19			
1	D	484	Total	C	N	O	S	0	0	0
			3741	2379	638	705	19			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q16881
A	-12	ALA	-	EXPRESSION TAG	UNP Q16881
A	-11	HIS	-	EXPRESSION TAG	UNP Q16881
A	-10	HIS	-	EXPRESSION TAG	UNP Q16881
A	-9	HIS	-	EXPRESSION TAG	UNP Q16881
A	-8	HIS	-	EXPRESSION TAG	UNP Q16881
A	-7	HIS	-	EXPRESSION TAG	UNP Q16881
A	-6	HIS	-	EXPRESSION TAG	UNP Q16881
A	-5	VAL	-	EXPRESSION TAG	UNP Q16881
A	-4	ASP	-	EXPRESSION TAG	UNP Q16881
A	-3	ASP	-	EXPRESSION TAG	UNP Q16881
A	-2	ASP	-	EXPRESSION TAG	UNP Q16881
A	-1	ASP	-	EXPRESSION TAG	UNP Q16881
A	498	CYS	U	SEE REMARK 999	UNP Q16881
B	-13	MET	-	EXPRESSION TAG	UNP Q16881
B	-12	ALA	-	EXPRESSION TAG	UNP Q16881
B	-11	HIS	-	EXPRESSION TAG	UNP Q16881
B	-10	HIS	-	EXPRESSION TAG	UNP Q16881
B	-9	HIS	-	EXPRESSION TAG	UNP Q16881
B	-8	HIS	-	EXPRESSION TAG	UNP Q16881
B	-7	HIS	-	EXPRESSION TAG	UNP Q16881

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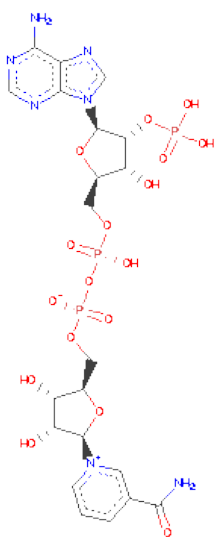
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP Q16881
B	-5	VAL	-	EXPRESSION TAG	UNP Q16881
B	-4	ASP	-	EXPRESSION TAG	UNP Q16881
B	-3	ASP	-	EXPRESSION TAG	UNP Q16881
B	-2	ASP	-	EXPRESSION TAG	UNP Q16881
B	-1	ASP	-	EXPRESSION TAG	UNP Q16881
B	498	CYS	U	SEE REMARK 999	UNP Q16881
C	-13	MET	-	EXPRESSION TAG	UNP Q16881
C	-12	ALA	-	EXPRESSION TAG	UNP Q16881
C	-11	HIS	-	EXPRESSION TAG	UNP Q16881
C	-10	HIS	-	EXPRESSION TAG	UNP Q16881
C	-9	HIS	-	EXPRESSION TAG	UNP Q16881
C	-8	HIS	-	EXPRESSION TAG	UNP Q16881
C	-7	HIS	-	EXPRESSION TAG	UNP Q16881
C	-6	HIS	-	EXPRESSION TAG	UNP Q16881
C	-5	VAL	-	EXPRESSION TAG	UNP Q16881
C	-4	ASP	-	EXPRESSION TAG	UNP Q16881
C	-3	ASP	-	EXPRESSION TAG	UNP Q16881
C	-2	ASP	-	EXPRESSION TAG	UNP Q16881
C	-1	ASP	-	EXPRESSION TAG	UNP Q16881
C	498	CYS	U	SEE REMARK 999	UNP Q16881
D	-13	MET	-	EXPRESSION TAG	UNP Q16881
D	-12	ALA	-	EXPRESSION TAG	UNP Q16881
D	-11	HIS	-	EXPRESSION TAG	UNP Q16881
D	-10	HIS	-	EXPRESSION TAG	UNP Q16881
D	-9	HIS	-	EXPRESSION TAG	UNP Q16881
D	-8	HIS	-	EXPRESSION TAG	UNP Q16881
D	-7	HIS	-	EXPRESSION TAG	UNP Q16881
D	-6	HIS	-	EXPRESSION TAG	UNP Q16881
D	-5	VAL	-	EXPRESSION TAG	UNP Q16881
D	-4	ASP	-	EXPRESSION TAG	UNP Q16881
D	-3	ASP	-	EXPRESSION TAG	UNP Q16881
D	-2	ASP	-	EXPRESSION TAG	UNP Q16881
D	-1	ASP	-	EXPRESSION TAG	UNP Q16881
D	498	CYS	U	SEE REMARK 999	UNP Q16881

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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 NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 4 is water.

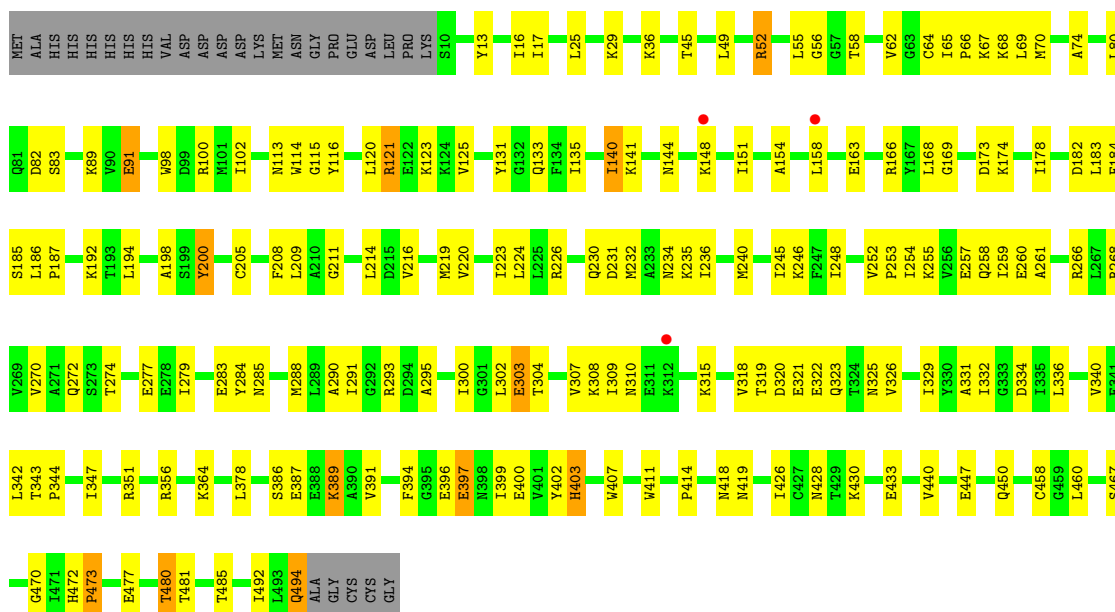
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total 246	O 246	0	0
4	B	260	Total 260	O 260	0	0
4	C	184	Total 184	O 184	0	0
4	D	207	Total 207	O 207	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($RSRZ > 2$). 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.

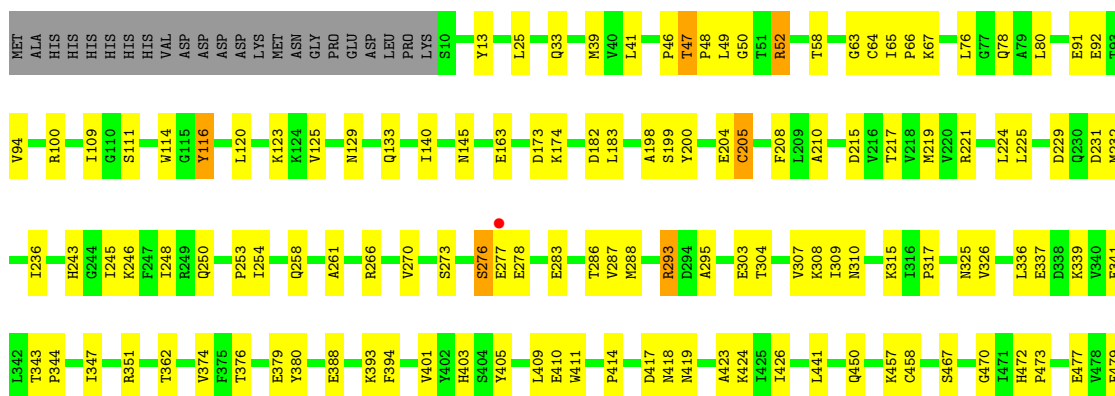
- Molecule 1: Thioredoxin reductase 1, cytoplasmic

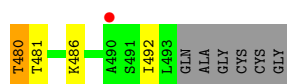
Chain A: 



- Molecule 1: Thioredoxin reductase 1, cytoplasmic

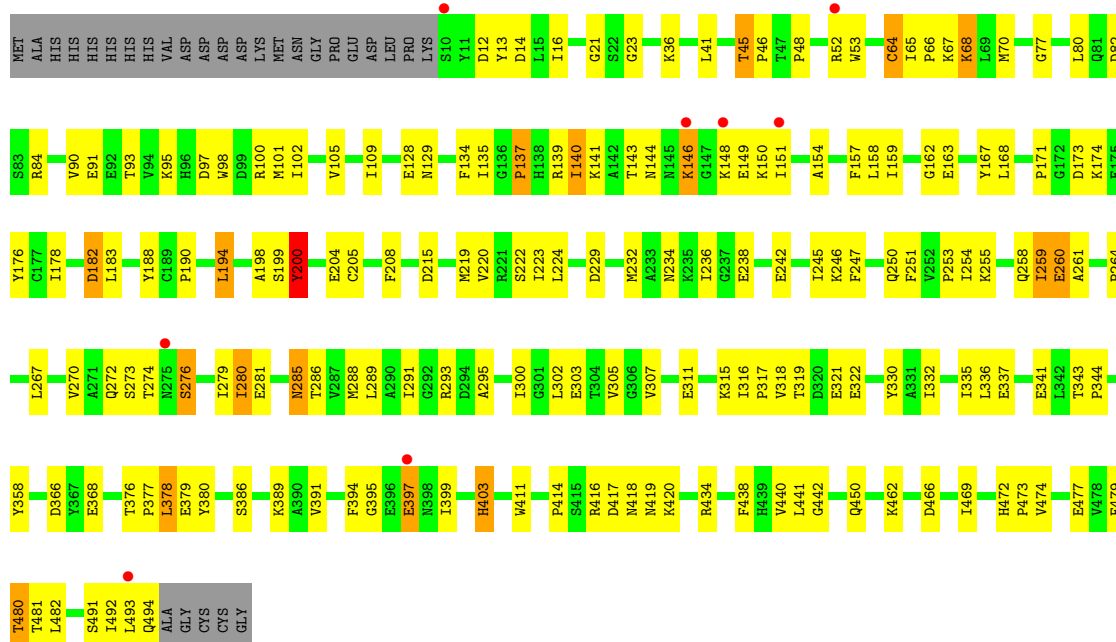
Chain B: 





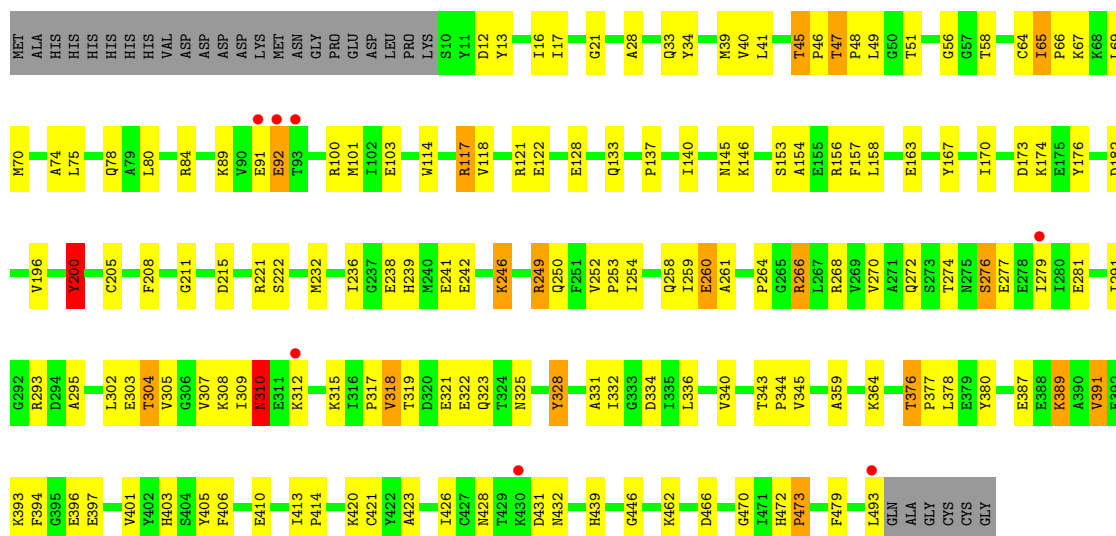
- Molecule 1: Thioredoxin reductase 1, cytoplasmic

Chain C:



- Molecule 1: Thioredoxin reductase 1, cytoplasmic

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	120.86Å 135.17Å 346.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.3 (30.00-2.60) 94.4 (29.92-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.260 0.210 , 0.259	Depositor DCC
R_{free} test set	4147 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 82282 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16283	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, 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	0.94	2/3824 (0.1%)	0.96	4/5178 (0.1%)
1	B	0.97	2/3815 (0.1%)	0.95	2/5166 (0.0%)
1	C	0.89	1/3824 (0.0%)	0.91	4/5178 (0.1%)
1	D	0.93	2/3815 (0.1%)	0.94	2/5166 (0.0%)
All	All	0.93	7/15278 (0.0%)	0.94	12/20688 (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	C	0	1
1	D	0	3
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	GLU	CG-CD	6.97	1.62	1.51
1	D	103	GLU	CG-CD	6.89	1.62	1.51
1	B	114	TRP	CB-CG	-6.17	1.39	1.50
1	D	397	GLU	CG-CD	5.87	1.60	1.51
1	C	53	TRP	CB-CG	-5.44	1.40	1.50
1	B	205	CYS	CB-SG	5.12	1.91	1.82
1	A	91	GLU	CB-CG	5.02	1.61	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	LEU	CA-CB-CG	-5.94	101.64	115.30
1	C	182	ASP	CB-CG-OD2	5.74	123.46	118.30
1	B	293	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	82	ASP	CB-CG-OD1	5.67	123.40	118.30
1	D	310	ASN	N-CA-C	-5.61	95.84	111.00
1	C	378	LEU	N-CA-C	-5.56	95.99	111.00
1	C	182	ASP	CB-CG-OD1	-5.38	113.45	118.30
1	A	100	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	B	310	ASN	N-CA-C	-5.29	96.73	111.00
1	D	65	ILE	C-N-CD	5.22	139.37	128.40
1	A	248	ILE	N-CA-C	-5.04	97.40	111.00
1	A	293	ARG	NE-CZ-NH1	-5.03	117.78	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	116	TYR	Sidechain
1	C	200	TYR	Sidechain
1	D	200	TYR	Sidechain
1	D	328	TYR	Sidechain
1	D	405	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3750	0	3759	151	0
1	B	3741	0	3751	110	0
1	C	3750	0	3759	167	0
1	D	3741	0	3751	134	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	2	0
3	A	48	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	25	4	0
3	C	48	0	25	3	0
3	D	48	0	25	3	0
4	A	246	0	0	5	0
4	B	260	0	0	7	0
4	C	184	0	0	5	0
4	D	207	0	0	1	0
All	All	16283	0	15244	534	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (534) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:308:LYS:N	1:B:325:ASN:HD21	1.43	1.17
1:C:419:ASN:ND2	1:C:494:GLN:HB2	1.62	1.13
1:D:302:LEU:HD22	1:D:307:VAL:HG21	1.27	1.12
1:B:308:LYS:H	1:B:325:ASN:ND2	1.48	1.09
1:C:183:LEU:HD22	1:C:288:MET:HE1	1.37	1.06
1:C:258:GLN:HE22	1:C:261:ALA:HB2	1.18	1.05
1:C:419:ASN:HD21	1:C:494:GLN:CB	1.69	1.05
1:C:311:GLU:OE2	4:C:702:HOH:O	1.77	1.01
1:D:39:MET:HE2	1:D:128:GLU:HG3	1.42	1.01
1:A:49:LEU:HD11	4:A:559:HOH:O	1.61	0.99
1:A:80:LEU:HD23	1:B:80:LEU:HD23	1.44	0.99
1:B:66:PRO:HG3	1:B:109:ILE:HD11	1.41	0.97
1:C:254:ILE:HD11	1:C:270:VAL:HG12	1.47	0.96
1:B:480:THR:HG22	1:B:481:THR:HG23	1.48	0.95
1:D:302:LEU:HD22	1:D:307:VAL:CG2	1.97	0.94
1:D:303:GLU:HG2	1:D:304:THR:N	1.84	0.93
1:D:39:MET:CE	1:D:128:GLU:HG3	1.99	0.92
1:C:493:LEU:O	1:C:493:LEU:HD12	1.70	0.92
1:C:285:ASN:HD22	1:C:285:ASN:N	1.68	0.92
1:A:36:LYS:HE2	1:A:36:LYS:HA	1.52	0.92
1:C:258:GLN:NE2	1:C:261:ALA:HB2	1.86	0.91
1:D:303:GLU:HG2	1:D:304:THR:H	1.38	0.89
1:D:84:ARG:NH1	1:D:92:GLU:HA	1.86	0.88
1:C:419:ASN:HD21	1:C:494:GLN:HB2	0.77	0.88
1:C:302:LEU:HD22	1:C:307:VAL:HB	1.56	0.88
1:C:318:VAL:HG11	1:C:322:GLU:HA	1.55	0.87
1:A:163:GLU:HG2	1:A:295:ALA:HA	1.56	0.85
1:D:47:THR:HG22	1:D:49:LEU:H	1.38	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:173:ASP:OD1	1:C:174:LYS:N	2.09	0.85
1:C:199:SER:OG	1:C:200:TYR:N	2.11	0.79
1:C:68:LYS:HE3	1:D:410:GLU:OE2	1.83	0.79
1:C:183:LEU:HD22	1:C:288:MET:CE	2.12	0.79
1:C:397:GLU:H	1:C:397:GLU:CD	1.84	0.78
1:C:258:GLN:HE21	1:C:261:ALA:N	1.81	0.78
1:C:254:ILE:CD1	1:C:270:VAL:HG12	2.14	0.77
1:C:254:ILE:HD11	1:C:270:VAL:CG1	2.14	0.77
1:A:121:ARG:HH11	1:A:121:ARG:CG	1.98	0.77
1:D:238:GLU:O	1:D:242:GLU:HG3	1.84	0.77
1:A:480:THR:HG22	1:A:481:THR:HG23	1.66	0.77
1:C:158:LEU:HD11	1:C:332:ILE:HG12	1.68	0.75
1:D:47:THR:HG22	1:D:49:LEU:N	2.00	0.75
1:C:168:LEU:HD23	1:C:291:ILE:HD13	1.69	0.74
1:B:100:ARG:HG2	1:B:100:ARG:HH21	1.51	0.74
1:A:70:MET:HE1	1:A:184:PHE:HD1	1.52	0.74
1:D:117:ARG:HG2	1:D:117:ARG:HH21	1.52	0.73
1:D:259:ILE:HD11	1:D:268:ARG:HB2	1.70	0.73
1:D:200:TYR:HB3	3:D:901:NAP:C5N	2.19	0.73
1:D:17:ILE:HG12	1:D:158:LEU:HD23	1.69	0.72
1:D:84:ARG:HH11	1:D:92:GLU:HA	1.52	0.72
1:A:67:LYS:C	1:A:67:LYS:HD2	2.09	0.72
1:B:215:ASP:OD1	1:B:246:LYS:NZ	2.23	0.72
1:C:67:LYS:HD2	1:C:67:LYS:C	2.10	0.72
1:B:258:GLN:OE1	1:B:261:ALA:HB2	1.90	0.72
1:A:200:TYR:HB3	3:A:901:NAP:C5N	2.20	0.71
1:B:200:TYR:HB3	3:B:901:NAP:C5N	2.20	0.71
1:C:394:PHE:HB2	1:C:399:ILE:HD11	1.73	0.71
1:B:405:TYR:CD1	1:B:492:ILE:HD13	2.25	0.70
1:C:41:LEU:HD23	1:C:128:GLU:HB2	1.73	0.70
1:A:173:ASP:OD1	1:A:174:LYS:N	2.25	0.70
1:C:16:ILE:HB	1:C:157:PHE:CE2	2.25	0.70
1:A:254:ILE:HD11	1:A:270:VAL:HG12	1.73	0.70
1:A:121:ARG:HH11	1:A:121:ARG:HG3	1.57	0.70
1:C:36:LYS:HE2	1:C:358:TYR:CD1	2.27	0.69
1:D:47:THR:CG2	1:D:49:LEU:H	2.05	0.69
1:A:266:ARG:NH1	1:A:283:GLU:OE1	2.22	0.69
1:B:250:GLN:HE22	1:D:222:SER:HB2	1.56	0.69
1:C:378:LEU:HD11	1:C:442:GLY:HA2	1.75	0.68
1:A:120:LEU:HD22	1:A:125:VAL:HG11	1.74	0.68
1:C:200:TYR:HB3	3:C:901:NAP:C5N	2.24	0.68
1:D:205:CYS:HA	1:D:208:PHE:CE2	2.28	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:LYS:HE2	1:A:36:LYS:CA	2.22	0.68
1:C:80:LEU:HD23	1:D:80:LEU:HD23	1.76	0.68
1:A:98:TRP:NE1	1:A:102:ILE:HG13	2.08	0.68
1:D:315:LYS:HE3	1:D:336:LEU:O	1.92	0.67
1:C:259:ILE:O	1:C:259:ILE:HG22	1.94	0.67
1:C:146:LYS:HE3	1:C:148:LYS:HE2	1.76	0.67
1:D:302:LEU:HB3	1:D:307:VAL:HG23	1.75	0.67
1:D:47:THR:HG21	1:D:182:ASP:OD1	1.94	0.67
1:A:70:MET:CE	1:A:184:PHE:HD1	2.07	0.67
1:C:474:VAL:O	1:C:477:GLU:HG2	1.95	0.67
1:A:80:LEU:HD23	1:B:80:LEU:CD2	2.23	0.66
1:C:254:ILE:CG1	1:C:270:VAL:HG12	2.24	0.66
1:A:194:LEU:HD22	1:A:284:TYR:CE1	2.29	0.66
1:C:168:LEU:CD2	1:C:291:ILE:HD13	2.25	0.66
1:C:70:MET:HG2	1:C:101:MET:HE3	1.77	0.66
1:B:315:LYS:HB2	1:B:337:GLU:HB2	1.76	0.66
1:B:205:CYS:HA	1:B:208:PHE:CE2	2.30	0.66
1:C:258:GLN:NE2	1:C:261:ALA:CB	2.56	0.66
1:C:238:GLU:O	1:C:242:GLU:HG3	1.94	0.66
1:A:121:ARG:NH1	1:A:121:ARG:HG3	2.09	0.66
1:C:379:GLU:O	1:C:441:LEU:HD12	1.96	0.66
1:C:198:ALA:HB2	1:C:220:VAL:HG13	1.78	0.66
1:A:319:THR:HG23	1:A:323:GLN:O	1.96	0.66
1:B:393:LYS:HD3	1:B:394:PHE:CE1	2.30	0.65
1:D:428:ASN:ND2	1:D:431:ASP:HB3	2.10	0.65
1:C:480:THR:HG22	1:C:481:THR:HG23	1.79	0.65
1:D:176:TYR:CE1	1:D:258:GLN:HB2	2.31	0.65
1:A:205:CYS:HA	1:A:208:PHE:CE2	2.32	0.65
1:C:258:GLN:NE2	1:C:261:ALA:CA	2.60	0.64
1:B:219:MET:SD	1:B:253:PRO:HD3	2.37	0.64
1:D:117:ARG:HG2	1:D:117:ARG:NH2	2.13	0.64
1:A:480:THR:CG2	1:A:481:THR:HG23	2.28	0.64
1:A:315:LYS:HD2	1:A:336:LEU:O	1.98	0.64
1:C:105:VAL:O	1:C:109:ILE:HG13	1.98	0.64
1:A:340:VAL:CG1	1:A:342:LEU:HD12	2.28	0.64
1:A:192:LYS:H	1:A:285:ASN:HD22	1.43	0.64
1:D:272:GLN:HB2	1:D:279:ILE:HD13	1.80	0.63
1:D:258:GLN:NE2	1:D:261:ALA:HA	2.14	0.63
1:A:400:GLU:HA	1:A:400:GLU:OE2	1.97	0.63
1:D:462:LYS:HD2	1:D:466:ASP:OD1	1.99	0.63
1:A:477:GLU:O	1:A:480:THR:HB	1.99	0.63
1:A:223:ILE:HD11	1:A:226:ARG:HB2	1.81	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:47:THR:HG21	1:B:182:ASP:OD1	1.99	0.62
1:B:47:THR:HG23	1:B:48:PRO:HD2	1.81	0.62
1:A:308:LYS:N	1:A:325:ASN:OD1	2.27	0.62
1:D:242:GLU:OE2	1:D:420:LYS:NZ	2.23	0.62
1:C:318:VAL:CG1	1:C:322:GLU:HA	2.27	0.62
1:A:472:HIS:ND1	1:A:473:PRO:HA	2.14	0.62
1:B:325:ASN:OD1	1:B:326:VAL:HG23	1.99	0.62
1:C:141:LYS:HD3	1:C:149:GLU:OE2	1.99	0.62
1:B:374:VAL:HG12	1:B:376:THR:HG23	1.81	0.62
1:A:318:VAL:HG23	1:A:323:GLN:C	2.21	0.61
1:C:171:PRO:CG	1:C:255:LYS:HD2	2.30	0.61
1:D:100:ARG:HG2	1:D:100:ARG:NH2	2.14	0.61
1:C:254:ILE:HG12	1:C:270:VAL:O	2.00	0.61
1:B:91:GLU:OE2	4:B:660:HOH:O	2.16	0.61
1:C:322:GLU:HG2	1:C:332:ILE:HG22	1.83	0.61
1:A:186:LEU:HD12	1:A:187:PRO:HD2	1.80	0.61
1:A:387:GLU:O	1:A:391:VAL:HG23	2.01	0.60
1:C:315:LYS:HD2	1:C:336:LEU:O	2.01	0.60
1:A:17:ILE:HG12	1:A:158:LEU:HD23	1.83	0.60
1:C:293:ARG:HG2	1:C:293:ARG:HH11	1.67	0.60
1:D:413:ILE:HB	1:D:414:PRO:HD3	1.83	0.60
1:A:209:LEU:HB3	1:A:214:LEU:HD12	1.84	0.59
1:A:80:LEU:CD2	1:B:80:LEU:HD23	2.26	0.59
1:C:163:GLU:HG2	1:C:295:ALA:HA	1.83	0.59
1:A:303:GLU:OE1	1:A:304:THR:HG23	2.02	0.59
1:D:305:VAL:CG2	1:D:328:TYR:OH	2.51	0.58
1:D:258:GLN:NE2	1:D:261:ALA:CA	2.66	0.58
1:D:254:ILE:HD11	1:D:270:VAL:HG12	1.83	0.58
1:D:387:GLU:O	1:D:391:VAL:HG12	2.03	0.58
1:C:293:ARG:HG2	1:C:293:ARG:NH1	2.17	0.58
1:C:178:ILE:HB	1:C:182:ASP:HB2	1.86	0.58
1:A:325:ASN:ND2	1:A:326:VAL:HG23	2.18	0.58
1:A:419:ASN:OD1	1:A:494:GLN:HB2	2.03	0.58
1:A:168:LEU:HD21	3:A:901:NAP:N6A	2.19	0.58
1:B:100:ARG:NH2	1:B:100:ARG:HG2	2.19	0.57
1:B:245:ILE:H	1:B:245:ILE:HD12	1.68	0.57
1:B:401:VAL:HG11	1:B:486:LYS:HD2	1.86	0.57
1:A:318:VAL:CG2	1:A:322:GLU:C	2.73	0.57
1:A:183:LEU:HD12	1:A:183:LEU:O	2.04	0.57
1:B:405:TYR:CE1	1:B:492:ILE:HD13	2.39	0.57
1:C:378:LEU:CD2	1:C:441:LEU:HG	2.35	0.57
1:D:272:GLN:OE1	1:D:279:ILE:HD11	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:270:VAL:HG22	1:D:281:GLU:HG2	1.87	0.57
1:C:98:TRP:NE1	1:C:102:ILE:HG13	2.20	0.57
1:C:36:LYS:HE2	1:C:358:TYR:HD1	1.70	0.57
1:A:394:PHE:HD2	1:A:430:LYS:HE2	1.70	0.57
1:D:156:ARG:HG3	1:D:156:ARG:HH11	1.70	0.57
1:C:234:ASN:O	1:C:238:GLU:HG3	2.05	0.57
1:A:351:ARG:HD3	4:A:723:HOH:O	2.05	0.57
1:B:92:GLU:HG2	1:B:92:GLU:O	2.05	0.57
1:C:137:PRO:O	1:C:139:ARG:HG3	2.04	0.56
1:C:250:GLN:HB3	1:C:274:THR:HG22	1.87	0.56
1:D:334:ASP:OD2	2:D:900:FAD:H5'1	2.05	0.56
1:D:41:LEU:HD23	1:D:128:GLU:HB2	1.88	0.56
1:A:234:ASN:ND2	4:A:699:HOH:O	2.37	0.56
1:C:417:ASP:HB3	1:C:420:LYS:HG3	1.87	0.56
1:A:343:THR:HB	1:A:344:PRO:HD3	1.87	0.56
1:B:424:LYS:HE3	1:B:426:ILE:HD11	1.87	0.56
1:D:309:ILE:HG13	1:D:310:ASN:N	2.20	0.56
1:D:91:GLU:HG2	1:D:92:GLU:N	2.21	0.56
1:A:472:HIS:HD1	1:A:473:PRO:HA	1.71	0.56
1:A:259:ILE:HG21	1:A:266:ARG:NH2	2.21	0.56
1:A:158:LEU:HD11	1:A:332:ILE:HG12	1.87	0.56
1:D:16:ILE:HD12	1:D:157:PHE:CZ	2.41	0.56
1:A:344:PRO:HG3	1:B:472:HIS:HB2	1.87	0.56
1:D:140:ILE:HG21	1:D:157:PHE:HE2	1.69	0.56
1:A:140:ILE:HG12	1:A:141:LYS:N	2.21	0.55
1:B:343:THR:HB	1:B:344:PRO:HD3	1.88	0.55
1:C:173:ASP:HB2	1:C:289:LEU:HD11	1.88	0.55
1:A:391:VAL:HG13	1:A:396:GLU:HA	1.86	0.55
1:B:173:ASP:OD1	1:B:174:LYS:N	2.37	0.55
1:B:405:TYR:HD1	1:B:492:ILE:HD13	1.72	0.55
1:C:70:MET:HG2	1:C:101:MET:CE	2.36	0.55
1:C:245:ILE:HG22	1:C:247:PHE:CE2	2.42	0.55
1:C:285:ASN:ND2	1:C:285:ASN:N	2.43	0.55
1:D:319:THR:HG23	1:D:323:GLN:O	2.07	0.55
1:C:477:GLU:O	1:C:480:THR:HB	2.07	0.55
1:D:428:ASN:ND2	1:D:431:ASP:CB	2.70	0.55
1:D:133:GLN:O	1:D:140:ILE:HG13	2.08	0.54
1:A:258:GLN:OE1	1:A:261:ALA:HB2	2.07	0.54
1:D:259:ILE:CD1	1:D:268:ARG:HB2	2.36	0.54
1:A:319:THR:C	1:A:321:GLU:H	2.10	0.54
1:B:308:LYS:HB2	1:B:325:ASN:HD22	1.72	0.54
1:D:423:ALA:HB1	1:D:479:PHE:CZ	2.43	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:133:GLN:O	1:B:140:ILE:HG13	2.08	0.54
1:B:308:LYS:HE2	1:B:325:ASN:HD22	1.72	0.53
1:C:259:ILE:O	1:C:260:GLU:CB	2.56	0.53
1:C:319:THR:C	1:C:321:GLU:H	2.11	0.53
1:A:318:VAL:HG21	1:A:322:GLU:C	2.29	0.53
1:C:258:GLN:HE21	1:C:261:ALA:CA	2.21	0.53
1:B:47:THR:HG22	1:B:49:LEU:H	1.72	0.53
1:A:428:ASN:OD1	1:A:430:LYS:HG2	2.08	0.53
1:B:273:SER:OG	1:B:278:GLU:HG2	2.08	0.53
1:A:340:VAL:HG12	1:A:342:LEU:HD12	1.89	0.53
1:D:17:ILE:HB	1:D:40:VAL:HG22	1.89	0.53
1:A:391:VAL:HG13	1:A:396:GLU:CA	2.39	0.53
1:A:236:ILE:O	1:A:240:MET:HG3	2.09	0.53
1:A:325:ASN:HD21	1:A:326:VAL:HG23	1.74	0.53
1:A:255:LYS:HE3	1:A:257:GLU:HB3	1.91	0.53
1:A:178:ILE:HB	1:A:182:ASP:HB2	1.89	0.53
1:C:302:LEU:HD22	1:C:307:VAL:CB	2.35	0.53
1:B:293:ARG:HD3	3:B:901:NAP:H51N	1.90	0.53
1:A:13:TYR:O	1:A:154:ALA:HA	2.08	0.53
1:B:379:GLU:O	1:B:441:LEU:HD12	2.09	0.53
1:D:293:ARG:HD3	3:D:901:NAP:H51N	1.90	0.52
1:C:95:LYS:CB	1:D:89:LYS:HE3	2.39	0.52
1:D:34:TYR:CE2	1:D:359:ALA:HB2	2.45	0.52
1:C:366:ASP:C	1:C:366:ASP:OD1	2.48	0.52
1:B:308:LYS:HB2	1:B:325:ASN:ND2	2.24	0.52
1:D:272:GLN:HB2	1:D:279:ILE:CD1	2.39	0.52
1:D:241:GLU:CD	1:D:249:ARG:HH22	2.13	0.52
1:C:322:GLU:O	1:C:330:TYR:HB3	2.10	0.52
1:B:217:THR:HG21	1:B:248:ILE:HD12	1.92	0.52
1:C:450:GLN:OE1	1:D:470:GLY:HA2	2.09	0.52
1:D:258:GLN:HE21	1:D:261:ALA:HA	1.73	0.52
1:C:84:ARG:HG2	1:C:90:VAL:HG23	1.91	0.52
1:C:90:VAL:HG11	1:D:80:LEU:CD2	2.40	0.52
1:C:134:PHE:CD1	1:C:305:VAL:HG11	2.45	0.52
1:C:343:THR:HB	1:C:344:PRO:HD3	1.92	0.52
1:C:480:THR:CG2	1:C:481:THR:HG23	2.40	0.51
1:B:33:GLN:HE21	1:B:123:LYS:NZ	2.09	0.51
1:A:223:ILE:HD11	1:A:226:ARG:CB	2.39	0.51
1:D:100:ARG:HH21	1:D:100:ARG:HG2	1.74	0.51
1:C:258:GLN:HG2	1:C:260:GLU:H	1.75	0.50
1:D:309:ILE:HA	1:D:317:PRO:HD2	1.93	0.50
1:D:389:LYS:HD3	1:D:389:LYS:N	2.25	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:462:LYS:HD2	1:C:462:LYS:O	2.11	0.50
1:C:135:ILE:HD13	1:C:151:ILE:HD12	1.94	0.50
1:A:29:LYS:HG2	1:A:123:LYS:HG3	1.93	0.50
1:D:114:TRP:HZ3	1:D:117:ARG:HH11	1.58	0.50
1:B:315:LYS:HE3	1:B:336:LEU:O	2.10	0.50
1:D:276:SER:OG	1:D:277:GLU:N	2.44	0.50
1:C:259:ILE:CG2	1:C:259:ILE:O	2.60	0.50
1:C:140:ILE:HG21	1:C:157:PHE:CE2	2.47	0.50
1:C:198:ALA:CB	1:C:220:VAL:HG13	2.41	0.50
1:A:472:HIS:HB2	1:B:344:PRO:HG3	1.94	0.50
1:D:322:GLU:HG2	1:D:332:ILE:HG22	1.94	0.50
1:A:318:VAL:HG22	1:A:319:THR:N	2.27	0.50
1:C:23:GLY:HA3	1:C:332:ILE:HD12	1.94	0.50
1:A:394:PHE:CD2	1:A:430:LYS:HE2	2.46	0.50
1:B:410:GLU:H	1:B:410:GLU:CD	2.15	0.50
1:A:331:ALA:C	1:A:336:LEU:HD21	2.31	0.50
1:B:307:VAL:HA	1:B:325:ASN:OD1	2.12	0.49
1:A:447:GLU:OE1	1:A:447:GLU:HA	2.13	0.49
1:A:274:THR:CG2	1:A:274:THR:O	2.60	0.49
1:D:70:MET:HG2	1:D:101:MET:CE	2.41	0.49
1:C:215:ASP:OD1	1:C:246:LYS:NZ	2.41	0.49
1:B:198:ALA:HB1	1:B:224:LEU:HD22	1.93	0.49
1:A:309:ILE:HG13	1:A:310:ASN:N	2.27	0.49
1:B:245:ILE:HD12	1:B:245:ILE:N	2.27	0.49
1:D:236:ILE:HD11	1:D:380:TYR:HB2	1.95	0.49
1:C:440:VAL:HG13	1:C:440:VAL:O	2.13	0.49
1:C:318:VAL:CG1	1:C:319:THR:N	2.76	0.49
1:D:406:PHE:CZ	1:D:421:CYS:HB3	2.48	0.49
1:C:251:PHE:CE1	1:C:280:ILE:HD12	2.48	0.49
1:B:47:THR:O	1:B:50:GLY:N	2.37	0.49
1:D:343:THR:HB	1:D:344:PRO:HD3	1.95	0.49
1:B:200:TYR:CD2	3:B:901:NAP:H3D	2.47	0.49
1:A:318:VAL:HG23	1:A:323:GLN:O	2.13	0.49
1:A:356:ARG:NH1	1:A:364:LYS:HA	2.28	0.48
1:C:143:THR:HG23	1:C:149:GLU:HG2	1.94	0.48
1:B:339:LYS:CE	4:B:783:HOH:O	2.60	0.48
1:D:260:GLU:OE1	1:D:266:ARG:NH2	2.46	0.48
1:B:405:TYR:CE1	1:B:492:ILE:CD1	2.96	0.48
1:A:214:LEU:O	1:A:216:VAL:HG23	2.13	0.48
1:B:65:ILE:HG22	1:B:66:PRO:N	2.28	0.48
1:D:75:LEU:O	1:D:78:GLN:HB3	2.14	0.48
1:B:46:PRO:HB3	1:B:52:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:258:GLN:HE21	1:C:260:GLU:C	2.16	0.48
1:D:12:ASP:HB2	1:D:153:SER:O	2.13	0.48
1:C:90:VAL:HG11	1:D:80:LEU:HD21	1.95	0.48
1:A:198:ALA:HB1	1:A:224:LEU:HD23	1.95	0.48
1:C:97:ASP:OD1	4:C:561:HOH:O	2.20	0.48
1:A:135:ILE:CD1	1:A:151:ILE:HD13	2.42	0.48
1:B:418:ASN:OD1	1:B:419:ASN:ND2	2.47	0.48
1:C:95:LYS:HB3	1:D:89:LYS:HE3	1.96	0.48
1:A:55:LEU:O	1:A:113:ASN:OD1	2.32	0.48
1:A:450:GLN:OE1	1:B:470:GLY:HA2	2.14	0.48
1:C:67:LYS:HD2	1:C:68:LYS:N	2.29	0.48
1:C:13:TYR:O	1:C:154:ALA:HA	2.14	0.48
1:C:198:ALA:HB1	1:C:224:LEU:CD2	2.43	0.48
1:A:272:GLN:HB2	1:A:279:ILE:HG12	1.95	0.48
1:B:308:LYS:CB	1:B:325:ASN:ND2	2.76	0.48
1:C:149:GLU:O	1:C:150:LYS:HG3	2.14	0.48
1:C:272:GLN:HB2	1:C:279:ILE:HD13	1.94	0.48
1:D:173:ASP:OD1	1:D:174:LYS:N	2.40	0.47
1:C:493:LEU:CD1	1:C:493:LEU:O	2.52	0.47
1:C:397:GLU:N	1:C:397:GLU:OE2	2.43	0.47
1:D:258:GLN:HE22	1:D:261:ALA:HB2	1.79	0.47
1:C:171:PRO:HG3	1:C:255:LYS:HD2	1.94	0.47
1:D:74:ALA:HB1	1:D:211:GLY:HA3	1.97	0.47
1:C:91:GLU:HG3	1:C:93:THR:H	1.78	0.47
1:C:474:VAL:HG11	1:D:446:GLY:HA3	1.96	0.47
1:B:47:THR:HG22	1:B:49:LEU:N	2.30	0.47
1:A:25:LEU:HD13	1:A:116:TYR:CD1	2.49	0.47
1:D:302:LEU:HB3	1:D:307:VAL:CG2	2.42	0.47
1:C:167:TYR:CE2	1:C:174:LYS:HA	2.50	0.47
1:A:98:TRP:CZ2	1:A:102:ILE:HD11	2.49	0.47
1:A:343:THR:O	1:A:347:ILE:HG13	2.14	0.47
1:A:232:MET:O	1:A:236:ILE:HG13	2.14	0.47
1:D:167:TYR:CE2	1:D:174:LYS:HA	2.50	0.47
1:D:232:MET:HE2	1:D:439:HIS:HB3	1.96	0.47
1:D:21:GLY:HA2	1:D:56:GLY:O	2.13	0.47
1:C:222:SER:OG	1:C:223:ILE:N	2.44	0.47
1:D:118:VAL:O	1:D:122:GLU:HG3	2.14	0.47
1:A:302:LEU:HD13	1:A:307:VAL:HG12	1.97	0.47
1:A:55:LEU:HD12	1:A:56:GLY:H	1.79	0.47
1:A:192:LYS:N	1:A:285:ASN:HD22	2.12	0.47
1:C:135:ILE:HD11	1:C:139:ARG:NH1	2.29	0.47
1:C:229:ASP:OD1	1:C:232:MET:HG2	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:340:VAL:HB	1:D:345:VAL:HG21	1.97	0.47
1:C:419:ASN:ND2	1:C:494:GLN:HE21	2.12	0.46
1:D:258:GLN:NE2	1:D:261:ALA:HB2	2.30	0.46
1:C:171:PRO:HG2	1:C:255:LYS:HD2	1.97	0.46
1:D:65:ILE:HG22	1:D:66:PRO:N	2.30	0.46
1:A:52:ARG:HG3	1:A:52:ARG:NH1	2.30	0.46
1:C:200:TYR:HB3	3:C:901:NAP:C4N	2.45	0.46
1:B:200:TYR:HD2	3:B:901:NAP:H3D	1.81	0.46
1:B:477:GLU:O	1:B:480:THR:HB	2.15	0.46
1:A:403:HIS:CE1	1:A:492:ILE:HD13	2.51	0.46
1:A:246:LYS:HE2	4:A:738:HOH:O	2.15	0.46
1:C:46:PRO:HG3	1:C:52:ARG:HG2	1.96	0.46
1:A:121:ARG:HH11	1:A:121:ARG:HG2	1.79	0.46
1:B:266:ARG:NH1	1:B:283:GLU:OE1	2.47	0.46
1:D:196:VAL:HG21	1:D:253:PRO:HG2	1.97	0.46
1:B:145:ASN:HB2	4:B:746:HOH:O	2.16	0.46
1:C:418:ASN:OD1	1:C:419:ASN:N	2.49	0.46
1:A:230:GLN:O	1:A:234:ASN:ND2	2.48	0.46
1:C:302:LEU:CD2	1:C:307:VAL:HB	2.35	0.46
1:B:76:LEU:HA	1:B:76:LEU:HD23	1.60	0.46
1:B:308:LYS:H	1:B:325:ASN:HD21	0.66	0.45
1:C:259:ILE:O	1:C:260:GLU:HB2	2.15	0.45
1:D:215:ASP:OD1	1:D:246:LYS:HE2	2.16	0.45
1:A:120:LEU:HD22	1:A:125:VAL:CG1	2.44	0.45
1:A:407:TRP:CD1	1:A:418:ASN:HA	2.52	0.45
1:D:196:VAL:HG12	1:D:291:ILE:CG2	2.46	0.45
1:A:386:SER:OG	1:A:389:LYS:HB2	2.17	0.45
1:B:236:ILE:HD11	1:B:380:TYR:HB2	1.98	0.45
1:A:458:CYS:CB	1:B:458:CYS:HB3	2.46	0.45
1:D:308:LYS:N	1:D:325:ASN:OD1	2.41	0.45
1:B:163:GLU:HG2	1:B:295:ALA:HA	1.98	0.45
1:B:303:GLU:HG2	1:B:304:THR:N	2.30	0.45
1:A:307:VAL:HA	1:A:325:ASN:OD1	2.15	0.45
1:D:13:TYR:O	1:D:154:ALA:HA	2.15	0.45
1:D:221:ARG:O	1:D:250:GLN:HA	2.16	0.45
1:A:268:ARG:NH2	4:A:619:HOH:O	2.49	0.45
1:B:347:ILE:O	1:B:351:ARG:HG3	2.16	0.45
1:A:266:ARG:HH11	1:A:266:ARG:HG2	1.81	0.45
1:A:186:LEU:HA	1:A:187:PRO:HD2	1.80	0.45
1:C:462:LYS:HE2	1:C:466:ASP:OD2	2.17	0.45
1:A:166:ARG:HB3	1:A:291:ILE:HD12	1.97	0.45
1:C:21:GLY:HA3	2:C:900:FAD:O5B	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:303:GLU:H	1:A:303:GLU:CD	2.19	0.45
1:A:440:VAL:O	1:A:440:VAL:HG13	2.17	0.45
1:B:120:LEU:HD22	1:B:125:VAL:HG11	1.99	0.45
1:D:303:GLU:CG	1:D:304:THR:N	2.68	0.45
1:D:114:TRP:HZ3	1:D:117:ARG:NH1	2.13	0.45
1:D:140:ILE:HG21	1:D:157:PHE:CE2	2.49	0.45
1:D:266:ARG:HG2	1:D:266:ARG:HH11	1.81	0.45
1:B:13:TYR:CE2	1:B:39:MET:HB2	2.52	0.45
1:C:67:LYS:HE2	1:C:67:LYS:HB3	1.73	0.45
1:C:440:VAL:HB	1:C:479:PHE:HZ	1.82	0.45
1:C:251:PHE:CZ	1:C:280:ILE:HD12	2.52	0.45
1:A:168:LEU:CD2	3:A:901:NAP:N6A	2.79	0.44
1:B:351:ARG:HD2	4:B:539:HOH:O	2.17	0.44
1:C:494:GLN:HG3	1:C:494:GLN:O	2.17	0.44
1:A:67:LYS:HD2	1:A:68:LYS:N	2.33	0.44
1:C:411:TRP:O	1:C:414:PRO:HD2	2.17	0.44
1:A:467:SER:OG	1:B:457:LYS:HD2	2.17	0.44
1:C:219:MET:SD	1:C:253:PRO:HG3	2.58	0.44
1:C:344:PRO:HG3	1:D:472:HIS:HB2	1.99	0.44
1:A:300:ILE:HD11	1:A:302:LEU:HD21	1.99	0.44
1:C:82:ASP:OD2	1:C:416:ARG:NH1	2.36	0.44
1:C:391:VAL:O	1:C:395:GLY:N	2.41	0.44
1:B:325:ASN:OD1	1:B:326:VAL:N	2.50	0.44
1:A:163:GLU:HG2	1:A:295:ALA:CA	2.39	0.44
1:A:351:ARG:HE	1:A:351:ARG:HB3	1.36	0.44
1:C:97:ASP:OD2	1:C:100:ARG:HB2	2.18	0.44
1:C:188:TYR:CE1	1:C:264:PRO:HB3	2.53	0.44
1:D:376:THR:O	1:D:377:PRO:C	2.56	0.44
1:B:411:TRP:O	1:B:414:PRO:HG2	2.18	0.44
1:A:318:VAL:CG2	1:A:323:GLN:N	2.80	0.44
1:C:417:ASP:HB3	1:C:420:LYS:CG	2.46	0.44
1:A:141:LYS:HE3	1:A:141:LYS:HB3	1.69	0.44
1:A:470:GLY:HA2	1:B:450:GLN:OE1	2.18	0.44
1:D:117:ARG:CG	1:D:117:ARG:HH21	2.28	0.44
1:D:322:GLU:HB3	1:D:331:ALA:O	2.18	0.44
1:C:318:VAL:HG12	1:C:319:THR:O	2.18	0.43
1:A:321:GLU:O	1:A:322:GLU:HB2	2.17	0.43
1:D:156:ARG:NH1	1:D:156:ARG:HG3	2.33	0.43
1:C:95:LYS:HB2	1:D:89:LYS:HE3	2.00	0.43
1:C:162:GLY:O	1:C:335:ILE:HG22	2.18	0.43
1:C:194:LEU:HA	1:C:194:LEU:HD12	1.67	0.43
1:C:199:SER:O	1:C:200:TYR:C	2.57	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:300:ILE:HG13	1:A:302:LEU:HG	2.00	0.43
1:A:83:SER:HA	1:B:76:LEU:HD13	2.01	0.43
1:A:402:TYR:CE2	1:A:485:THR:HG22	2.53	0.43
1:C:65:ILE:HB	1:C:66:PRO:CD	2.48	0.43
1:A:49:LEU:HD12	1:A:49:LEU:H	1.83	0.43
1:A:303:GLU:OE1	1:A:304:THR:CG2	2.67	0.43
1:B:254:ILE:CG1	1:B:270:VAL:HG12	2.47	0.43
1:D:428:ASN:HD21	1:D:431:ASP:HB2	1.83	0.43
1:C:236:ILE:HD11	1:C:380:TYR:CD2	2.53	0.43
1:B:199:SER:HA	1:B:225:LEU:HD23	1.99	0.43
1:A:133:GLN:NE2	1:A:141:LYS:NZ	2.67	0.43
1:B:67:LYS:HD3	1:B:204:GLU:OE1	2.18	0.43
1:C:273:SER:OG	1:C:276:SER:N	2.46	0.43
1:C:394:PHE:HB2	1:C:399:ILE:CD1	2.46	0.43
1:B:339:LYS:NZ	4:B:783:HOH:O	2.45	0.43
1:C:188:TYR:CD1	1:C:188:TYR:C	2.92	0.43
1:C:258:GLN:NE2	1:C:261:ALA:N	2.57	0.43
1:C:378:LEU:HD12	1:C:378:LEU:HA	1.72	0.43
1:D:176:TYR:CD1	1:D:258:GLN:HB2	2.53	0.43
1:C:163:GLU:HG2	1:C:295:ALA:CA	2.49	0.43
1:D:39:MET:HE1	1:D:128:GLU:HG3	1.94	0.43
1:A:231:ASP:O	1:A:235:LYS:HG3	2.19	0.43
1:B:47:THR:HG23	1:B:48:PRO:CD	2.49	0.43
1:A:472:HIS:CE1	1:A:473:PRO:HB3	2.54	0.43
1:D:254:ILE:HD11	1:D:270:VAL:CG1	2.49	0.43
1:C:472:HIS:HB2	1:D:344:PRO:HG3	2.00	0.43
1:B:423:ALA:HB1	1:B:479:PHE:CE1	2.53	0.43
1:B:470:GLY:H	1:B:480:THR:HG21	1.85	0.42
1:C:190:PRO:O	1:C:286:THR:OG1	2.32	0.42
1:D:252:VAL:HG13	3:D:901:NAP:N1A	2.34	0.42
1:B:47:THR:O	1:B:48:PRO:C	2.58	0.42
1:C:176:TYR:HB3	1:C:267:LEU:HD21	2.00	0.42
1:A:58:THR:HG23	1:A:62:VAL:HG23	2.01	0.42
1:D:393:LYS:HE2	1:D:394:PHE:CZ	2.54	0.42
1:D:472:HIS:HA	1:D:473:PRO:HA	1.81	0.42
1:B:210:ALA:CB	1:B:245:ILE:HD11	2.50	0.42
1:A:144:ASN:HD21	1:A:148:LYS:HB2	1.83	0.42
1:A:98:TRP:HE1	1:A:102:ILE:HG13	1.84	0.42
1:A:240:MET:HE2	1:A:245:ILE:HD13	2.01	0.42
1:B:411:TRP:CE3	1:B:417:ASP:HB2	2.55	0.42
1:B:25:LEU:HD13	1:B:116:TYR:CD1	2.54	0.42
1:B:229:ASP:OD1	1:B:232:MET:HG2	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:68:LYS:HE2	1:D:473:PRO:O	2.20	0.42
1:B:215:ASP:CG	1:B:246:LYS:HZ1	2.19	0.42
1:C:198:ALA:HB1	1:C:224:LEU:HD23	2.00	0.42
1:A:418:ASN:ND2	1:A:419:ASN:H	2.17	0.42
1:D:65:ILE:O	1:D:69:LEU:HG	2.19	0.42
1:D:302:LEU:CD2	1:D:307:VAL:CG2	2.85	0.42
1:B:100:ARG:NH2	1:B:100:ARG:CG	2.83	0.42
1:C:366:ASP:OD1	1:C:368:GLU:N	2.45	0.42
1:A:219:MET:SD	1:A:253:PRO:HD3	2.59	0.42
1:B:100:ARG:NH2	4:B:602:HOH:O	2.53	0.42
1:B:405:TYR:HE1	1:B:492:ILE:CD1	2.32	0.42
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.85	0.42
1:A:397:GLU:CD	1:A:397:GLU:H	2.23	0.42
1:A:411:TRP:C	1:A:414:PRO:HD2	2.39	0.42
1:A:458:CYS:HB3	1:B:458:CYS:HB3	2.02	0.42
1:A:288:MET:CE	1:A:290:ALA:HB2	2.49	0.42
1:D:163:GLU:HG2	1:D:295:ALA:HA	2.02	0.42
1:D:146:LYS:O	1:D:146:LYS:HE2	2.20	0.42
1:A:307:VAL:HG21	1:A:329:ILE:HG21	2.01	0.41
1:C:45:THR:HG23	4:C:813:HOH:O	2.19	0.41
1:D:170:ILE:O	1:D:170:ILE:HG13	2.19	0.41
1:A:91:GLU:H	1:A:91:GLU:CD	2.23	0.41
1:D:318:VAL:HG22	1:D:323:GLN:N	2.35	0.41
1:C:438:PHE:CE2	1:C:479:PHE:CE1	3.08	0.41
1:B:243:HIS:CD2	4:B:625:HOH:O	2.72	0.41
1:C:386:SER:H	1:C:389:LYS:HE2	1.85	0.41
1:D:47:THR:HB	1:D:51:THR:H	1.85	0.41
1:D:137:PRO:HA	1:D:305:VAL:HG23	2.01	0.41
1:B:286:THR:HG22	1:B:287:VAL:N	2.36	0.41
1:C:377:PRO:HD2	4:C:569:HOH:O	2.19	0.41
1:C:67:LYS:HD3	1:C:204:GLU:OE1	2.21	0.41
1:B:221:ARG:O	1:B:250:GLN:HA	2.21	0.41
1:C:134:PHE:N	1:C:300:ILE:O	2.52	0.41
1:A:131:TYR:C	1:A:131:TYR:CD2	2.94	0.41
1:C:341:GLU:HB2	3:C:901:NAP:O2D	2.19	0.41
1:C:77:GLY:HA2	1:C:80:LEU:HD12	2.03	0.41
1:B:58:THR:O	1:B:63:GLY:N	2.53	0.41
1:C:321:GLU:O	1:C:322:GLU:HB2	2.20	0.41
1:D:67:LYS:HB3	1:D:67:LYS:HE2	1.81	0.41
1:B:309:ILE:HA	1:B:317:PRO:HD2	2.02	0.41
1:D:310:ASN:OD1	1:D:312:LYS:HB3	2.20	0.41
1:C:482:LEU:HB2	4:C:878:HOH:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:205:CYS:HA	1:C:208:PHE:CE2	2.56	0.41
1:A:169:GLY:N	1:A:173:ASP:OD2	2.50	0.41
1:A:133:GLN:CD	1:A:141:LYS:HZ2	2.24	0.41
1:D:239:HIS:CE1	1:D:378:LEU:HB2	2.56	0.41
1:C:258:GLN:C	1:C:260:GLU:H	2.24	0.41
1:D:318:VAL:HG22	1:D:322:GLU:C	2.41	0.41
1:D:319:THR:C	1:D:321:GLU:H	2.23	0.41
1:D:446:GLY:N	4:D:551:HOH:O	2.36	0.41
1:C:251:PHE:CD2	1:C:273:SER:HA	2.56	0.41
1:B:229:ASP:OD1	1:B:231:ASP:HB3	2.20	0.41
1:C:403:HIS:CE1	1:C:492:ILE:HD13	2.55	0.41
1:D:401:VAL:HG22	1:D:426:ILE:HG13	2.02	0.41
1:A:89:LYS:O	1:B:94:VAL:HG13	2.20	0.41
1:A:70:MET:SD	1:A:208:PHE:CE1	3.14	0.41
1:A:315:LYS:HE3	1:A:334:ASP:O	2.21	0.41
1:C:315:LYS:O	1:C:317:PRO:HD3	2.21	0.41
1:B:276:SER:OG	1:B:277:GLU:N	2.53	0.41
1:D:45:THR:HA	1:D:46:PRO:HD3	1.71	0.41
1:A:318:VAL:HG21	1:A:322:GLU:HA	2.02	0.40
1:C:469:ILE:HG22	1:D:344:PRO:HB2	2.02	0.40
1:A:460:LEU:HD12	1:B:458:CYS:SG	2.62	0.40
1:C:159:ILE:HD12	1:C:316:ILE:HD13	2.03	0.40
1:B:183:LEU:HD22	1:B:288:MET:SD	2.61	0.40
1:A:114:TRP:O	1:A:115:GLY:C	2.59	0.40
1:D:493:LEU:HD12	1:D:493:LEU:H	1.87	0.40
1:A:69:LEU:HD21	1:B:409:LEU:HG	2.03	0.40
1:D:332:ILE:HA	1:D:336:LEU:HD11	2.03	0.40
1:D:16:ILE:HG13	1:D:154:ALA:HB2	2.02	0.40
1:B:198:ALA:HB1	1:B:224:LEU:CD2	2.51	0.40
1:A:198:ALA:CB	1:A:220:VAL:HG13	2.51	0.40
1:C:67:LYS:CD	1:C:67:LYS:C	2.82	0.40
1:B:258:GLN:OE1	1:B:261:ALA:CB	2.67	0.40
1:C:315:LYS:HB3	1:C:337:GLU:HB2	2.03	0.40
1:B:217:THR:CG2	1:B:248:ILE:HD12	2.51	0.40
1:B:229:ASP:HA	1:B:388:GLU:OE1	2.21	0.40
1:A:74:ALA:HB1	1:A:211:GLY:HA3	2.03	0.40
1:A:378:LEU:HA	1:A:378:LEU:HD12	1.80	0.40
1:B:41:LEU:HD23	1:B:41:LEU:HA	1.86	0.40
1:A:67:LYS:HE2	1:A:67:LYS:HB3	1.84	0.40
1:D:58:THR:OG1	2:D:900:FAD:O2A	2.18	0.40
1:A:399:ILE:HG23	1:A:426:ILE:HG23	2.04	0.40
1:A:65:ILE:HB	1:A:66:PRO:CD	2.52	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:28:ALA:HB2	1:D:40:VAL:HG21	2.04	0.40
1:D:100:ARG:HH21	1:D:100:ARG:CG	2.33	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	483/513 (94%)	446 (92%)	33 (7%)	4 (1%)	27	53
1	B	482/513 (94%)	455 (94%)	26 (5%)	1 (0%)	56	82
1	C	483/513 (94%)	443 (92%)	34 (7%)	6 (1%)	19	39
1	D	482/513 (94%)	443 (92%)	36 (8%)	3 (1%)	33	63
All	All	1930/2052 (94%)	1787 (93%)	129 (7%)	14 (1%)	30	58

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	260	GLU
1	A	200	TYR
1	C	200	TYR
1	D	260	GLU
1	A	260	GLU
1	A	320	ASP
1	D	200	TYR
1	B	473	PRO
1	C	64	CYS
1	C	137	PRO
1	C	259	ILE
1	A	473	PRO
1	C	473	PRO
1	D	473	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	399/422 (94%)	383 (96%)	16 (4%)	42	73
1	B	398/422 (94%)	386 (97%)	12 (3%)	53	82
1	C	399/422 (94%)	378 (95%)	21 (5%)	32	58
1	D	398/422 (94%)	373 (94%)	25 (6%)	25	49
All	All	1594/1688 (94%)	1520 (95%)	74 (5%)	37	66

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	45	THR
1	A	52	ARG
1	A	64	CYS
1	A	121	ARG
1	A	140	ILE
1	A	185	SER
1	A	252	VAL
1	A	277	GLU
1	A	303	GLU
1	A	389	LYS
1	A	397	GLU
1	A	403	HIS
1	A	433	GLU
1	A	480	THR
1	A	494	GLN
1	B	47	THR
1	B	52	ARG
1	B	64	CYS
1	B	78	GLN
1	B	111	SER
1	B	129	ASN
1	B	276	SER
1	B	341	GLU
1	B	362	THR
1	B	403	HIS

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Mol	Chain	Res	Type
1	B	467	SER
1	B	480	THR
1	C	12	ASP
1	C	14	ASP
1	C	45	THR
1	C	48	PRO
1	C	64	CYS
1	C	68	LYS
1	C	129	ASN
1	C	140	ILE
1	C	144	ASN
1	C	146	LYS
1	C	276	SER
1	C	280	ILE
1	C	281	GLU
1	C	285	ASN
1	C	303	GLU
1	C	376	THR
1	C	397	GLU
1	C	403	HIS
1	C	434	ARG
1	C	480	THR
1	C	491	SER
1	D	33	GLN
1	D	45	THR
1	D	47	THR
1	D	48	PRO
1	D	64	CYS
1	D	92	GLU
1	D	117	ARG
1	D	121	ARG
1	D	145	ASN
1	D	246	LYS
1	D	249	ARG
1	D	264	PRO
1	D	266	ARG
1	D	274	THR
1	D	276	SER
1	D	304	THR
1	D	310	ASN
1	D	318	VAL
1	D	364	LYS

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Mol	Chain	Res	Type
1	D	376	THR
1	D	389	LYS
1	D	391	VAL
1	D	396	GLU
1	D	403	HIS
1	D	432	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	113	ASN
1	A	129	ASN
1	A	133	GLN
1	A	234	ASN
1	A	285	ASN
1	A	418	ASN
1	B	33	GLN
1	B	107	ASN
1	B	113	ASN
1	B	129	ASN
1	B	145	ASN
1	B	250	GLN
1	B	419	ASN
1	B	432	ASN
1	C	85	ASN
1	C	113	ASN
1	C	129	ASN
1	C	145	ASN
1	C	258	GLN
1	C	272	GLN
1	C	285	ASN
1	C	419	ASN
1	C	494	GLN
1	D	81	GLN
1	D	129	ASN
1	D	145	ASN
1	D	250	GLN
1	D	258	GLN
1	D	355	GLN
1	D	419	ASN
1	D	428	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	$\# Z > 2$
2	FAD	A	900	-	58,58,58	1.60	6 (10%)	85,89,89	2.13	18 (21%)
3	NAP	A	901	-	52,52,52	1.47	6 (11%)	80,80,80	1.16	5 (6%)
2	FAD	B	900	-	58,58,58	1.63	10 (17%)	85,89,89	2.16	16 (18%)
3	NAP	B	901	-	52,52,52	1.49	8 (15%)	80,80,80	1.29	7 (8%)
2	FAD	C	900	-	58,58,58	1.79	9 (15%)	85,89,89	2.17	18 (21%)
3	NAP	C	901	-	52,52,52	1.52	9 (17%)	80,80,80	1.21	6 (7%)
2	FAD	D	900	-	58,58,58	1.74	7 (12%)	85,89,89	1.98	18 (21%)
3	NAP	D	901	-	52,52,52	1.35	7 (13%)	80,80,80	1.20	4 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	900	-	-	0/34/50/50	0/1/6/6
3	NAP	A	901	-	-	0/35/67/67	0/3/5/5
2	FAD	B	900	-	-	0/34/50/50	0/1/6/6
3	NAP	B	901	-	-	0/35/67/67	0/3/5/5
2	FAD	C	900	-	-	0/34/50/50	0/1/6/6
3	NAP	C	901	-	-	0/35/67/67	0/3/5/5
2	FAD	D	900	-	-	0/34/50/50	0/1/6/6
3	NAP	D	901	-	-	0/35/67/67	0/3/5/5

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	FAD	C4X-C10	6.18	1.51	1.40
2	B	900	FAD	C4-C4X	5.65	1.50	1.41
2	D	900	FAD	C4-C4X	5.30	1.49	1.41
2	C	900	FAD	C4-C4X	5.24	1.49	1.41
3	B	901	NAP	C2N-N1N	5.20	1.42	1.35
2	C	900	FAD	C4X-C10	5.08	1.49	1.40
2	D	900	FAD	C4X-C10	4.97	1.49	1.40
2	D	900	FAD	C9A-N10	4.96	1.46	1.38
2	C	900	FAD	C1'-C2'	4.52	1.55	1.51
2	C	900	FAD	C9A-N10	4.50	1.45	1.38
2	B	900	FAD	O4B-C1B	4.45	1.48	1.41
3	A	901	NAP	O4B-C1B	4.25	1.47	1.41
3	C	901	NAP	C2N-N1N	4.25	1.40	1.35
2	D	900	FAD	PA-O3P	4.19	1.67	1.59
2	A	900	FAD	C9A-N10	4.14	1.45	1.38
2	C	900	FAD	O4B-C1B	4.11	1.47	1.41
3	A	901	NAP	C4N-C3N	4.01	1.46	1.39
3	A	901	NAP	C2N-N1N	3.99	1.40	1.35
3	C	901	NAP	C4A-N3A	3.87	1.41	1.35
2	D	900	FAD	O4B-C1B	3.76	1.47	1.41
2	A	900	FAD	O4-C4	-3.74	1.17	1.24
3	C	901	NAP	O4B-C1B	3.73	1.47	1.41
3	B	901	NAP	O4B-C1B	3.71	1.47	1.41
2	A	900	FAD	O4B-C1B	3.61	1.46	1.41
3	C	901	NAP	C4N-C3N	3.60	1.45	1.39
2	B	900	FAD	C8A-N7A	-3.37	1.28	1.34
2	C	900	FAD	C8A-N7A	-3.33	1.28	1.34
2	B	900	FAD	C6-C5X	3.28	1.45	1.41
3	A	901	NAP	C6N-N1N	3.25	1.44	1.35
2	A	900	FAD	C4-C4X	3.22	1.46	1.41
3	D	901	NAP	C2N-N1N	3.18	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	901	NAP	C4N-C3N	3.09	1.44	1.39
2	A	900	FAD	C8A-N7A	-3.09	1.28	1.34
3	B	901	NAP	C4N-C3N	3.05	1.44	1.39
2	D	900	FAD	C8A-N7A	-3.00	1.28	1.34
3	D	901	NAP	O4B-C1B	3.00	1.46	1.41
3	D	901	NAP	C4A-N3A	2.96	1.40	1.35
3	C	901	NAP	C6N-N1N	2.95	1.43	1.35
3	B	901	NAP	C6N-N1N	2.94	1.43	1.35
2	D	900	FAD	C2B-C1B	-2.93	1.49	1.53
2	B	900	FAD	C2B-C1B	-2.87	1.49	1.53
3	B	901	NAP	C3N-C7N	2.76	1.55	1.50
3	B	901	NAP	C2A-N3A	2.72	1.37	1.32
2	B	900	FAD	C8A-N9A	2.72	1.40	1.36
2	B	900	FAD	C2-N3	-2.71	1.32	1.37
2	B	900	FAD	C4X-C10	2.69	1.45	1.40
3	C	901	NAP	C2A-N3A	2.56	1.37	1.32
3	D	901	NAP	C6N-N1N	2.55	1.42	1.35
3	A	901	NAP	C4A-N9A	-2.54	1.34	1.37
2	C	900	FAD	C2B-C1B	-2.47	1.49	1.53
2	C	900	FAD	C1'-N10	2.44	1.50	1.48
2	B	900	FAD	P-O1P	-2.40	1.42	1.51
3	B	901	NAP	C2B-C1B	-2.39	1.48	1.52
3	C	901	NAP	C3N-C7N	2.38	1.54	1.50
2	C	900	FAD	PA-O3P	2.34	1.64	1.59
3	B	901	NAP	O3B-C3B	2.33	1.48	1.43
3	C	901	NAP	PA-O3	2.30	1.64	1.59
3	A	901	NAP	C2A-N3A	2.28	1.36	1.32
3	C	901	NAP	P2B-O2B	2.27	1.66	1.59
3	D	901	NAP	O3B-C3B	2.25	1.48	1.43
3	D	901	NAP	C2A-N3A	2.10	1.36	1.32
2	B	900	FAD	C4X-N5	-2.02	1.31	1.36

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	FAD	N3A-C2A-N1A	-8.93	121.25	128.71
2	A	900	FAD	N3A-C2A-N1A	-8.90	121.27	128.71
2	B	900	FAD	N3A-C2A-N1A	-8.45	121.65	128.71
2	B	900	FAD	C2-N1-C10	7.21	122.25	114.98
2	A	900	FAD	P-O3P-PA	-6.94	111.34	131.68
2	D	900	FAD	N3A-C2A-N1A	-6.86	122.97	128.71
2	C	900	FAD	C2-N1-C10	6.80	121.83	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	FAD	C2-N1-C10	6.58	121.61	114.98
2	B	900	FAD	C4X-N5-C5X	6.32	123.79	116.69
2	A	900	FAD	C2-N1-C10	6.01	121.03	114.98
2	C	900	FAD	P-O3P-PA	-5.97	114.19	131.68
2	B	900	FAD	P-O3P-PA	-5.89	114.40	131.68
2	D	900	FAD	P-O3P-PA	-5.79	114.69	131.68
2	C	900	FAD	N3A-C4A-N9A	5.30	135.00	125.43
2	B	900	FAD	C4X-C10-N1	-5.26	117.47	122.73
2	D	900	FAD	C4X-N5-C5X	5.26	122.60	116.69
3	C	901	NAP	N3A-C2A-N1A	-5.21	124.35	128.71
2	A	900	FAD	C4X-C10-N10	-5.13	117.95	120.51
2	A	900	FAD	N3A-C4A-N9A	4.98	134.43	125.43
2	B	900	FAD	N3A-C4A-N9A	4.92	134.32	125.43
3	B	901	NAP	N3A-C2A-N1A	-4.86	124.64	128.71
3	D	901	NAP	N3A-C2A-N1A	-4.81	124.69	128.71
2	A	900	FAD	C4X-N5-C5X	4.80	122.09	116.69
2	D	900	FAD	N3A-C4A-N9A	4.78	134.07	125.43
3	A	901	NAP	N3A-C2A-N1A	-4.71	124.77	128.71
2	C	900	FAD	C4X-N5-C5X	4.66	121.92	116.69
2	B	900	FAD	C4X-C10-N10	-4.57	118.23	120.51
2	C	900	FAD	C2'-C1'-N10	-4.42	106.59	112.45
2	C	900	FAD	C4X-C10-N1	-3.95	118.78	122.73
2	D	900	FAD	C1'-N10-C9A	3.91	122.68	118.87
2	C	900	FAD	C1'-N10-C9A	3.85	122.61	118.87
2	C	900	FAD	C4B-O4B-C1B	-3.84	105.58	109.75
3	B	901	NAP	O4B-C1B-N9A	-3.83	104.88	108.44
2	C	900	FAD	C9A-N10-C10	-3.72	118.11	121.77
2	D	900	FAD	C4X-C10-N10	-3.67	118.68	120.51
2	A	900	FAD	C4X-C10-N1	-3.61	119.12	122.73
2	C	900	FAD	C4X-C10-N10	-3.57	118.73	120.51
2	D	900	FAD	C4X-C10-N1	-3.39	119.35	122.73
3	B	901	NAP	C6N-N1N-C2N	-3.34	118.26	122.04
2	B	900	FAD	O4B-C1B-C2B	-3.23	101.83	106.77
2	B	900	FAD	N1-C10-N10	3.17	124.30	115.97
2	D	900	FAD	O4B-C1B-C2B	-3.17	101.92	106.77
2	A	900	FAD	C4A-C5A-N7A	-3.09	106.88	109.52
2	C	900	FAD	O4B-C1B-C2B	-3.02	102.14	106.77
2	C	900	FAD	C5X-C9A-N10	3.01	119.77	116.80
2	D	900	FAD	C4A-C5A-N7A	-3.01	106.95	109.52
2	A	900	FAD	C4B-O4B-C1B	-2.95	106.55	109.75
2	A	900	FAD	C9A-N10-C10	-2.92	118.91	121.77
2	A	900	FAD	C1'-N10-C9A	2.88	121.67	118.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	FAD	C5X-C9A-N10	2.86	119.62	116.80
3	C	901	NAP	C6N-N1N-C2N	-2.86	118.81	122.04
3	D	901	NAP	C6N-N1N-C2N	-2.85	118.82	122.04
3	C	901	NAP	P2B-O2B-C2B	2.79	127.83	121.96
2	B	900	FAD	C9A-N10-C10	-2.76	119.06	121.77
2	A	900	FAD	O4B-C1B-C2B	-2.74	102.57	106.77
2	D	900	FAD	C5X-C9A-N10	2.70	119.46	116.80
2	D	900	FAD	O4B-C1B-N9A	-2.67	105.96	108.44
2	C	900	FAD	C5A-C4A-N3A	-2.67	119.89	125.70
3	B	901	NAP	P2B-O2B-C2B	2.66	127.55	121.96
2	A	900	FAD	N1-C10-N10	2.65	122.93	115.97
2	C	900	FAD	C4A-C5A-N7A	-2.65	107.25	109.52
2	B	900	FAD	C5X-C9A-N10	2.64	119.40	116.80
3	A	901	NAP	C6N-N1N-C2N	-2.60	119.10	122.04
2	D	900	FAD	C5A-C4A-N3A	-2.57	120.11	125.70
2	D	900	FAD	C9A-N10-C10	-2.55	119.27	121.77
2	C	900	FAD	C2A-N3A-C4A	2.55	121.27	114.01
3	B	901	NAP	O3B-C3B-C4B	-2.52	103.65	111.08
2	A	900	FAD	C5A-C4A-N3A	-2.49	120.28	125.70
2	C	900	FAD	N1-C10-N10	2.48	122.48	115.97
2	A	900	FAD	C2A-N3A-C4A	2.43	120.93	114.01
2	B	900	FAD	C4B-O4B-C1B	-2.39	107.16	109.75
2	B	900	FAD	C5A-C4A-N3A	-2.37	120.55	125.70
2	D	900	FAD	N1-C10-N10	2.28	121.95	115.97
3	D	901	NAP	C2A-N1A-C6A	2.27	122.88	118.77
3	A	901	NAP	C2A-N1A-C6A	2.24	122.81	118.77
2	B	900	FAD	C2A-N3A-C4A	2.21	120.30	114.01
2	A	900	FAD	C2'-C1'-N10	-2.20	109.53	112.45
3	C	901	NAP	C2A-N1A-C6A	2.19	122.72	118.77
3	C	901	NAP	C4A-C5A-N7A	2.16	111.37	109.52
2	D	900	FAD	C2A-N3A-C4A	2.13	120.07	114.01
2	A	900	FAD	C8A-N7A-C5A	2.11	110.13	103.58
3	B	901	NAP	O2X-P2B-O1X	2.09	117.28	110.44
2	D	900	FAD	C4B-O4B-C1B	-2.09	107.48	109.75
2	B	900	FAD	C4-N3-C2	-2.08	121.12	125.39
2	B	900	FAD	C4A-C5A-N7A	-2.08	107.74	109.52
3	A	901	NAP	C8A-N9A-C4A	-2.07	105.32	106.90
3	D	901	NAP	C4B-O4B-C1B	-2.05	107.52	109.75
2	D	900	FAD	C8A-N7A-C5A	2.05	109.94	103.58
3	B	901	NAP	C4A-C5A-N7A	2.03	111.26	109.52
2	C	900	FAD	C8A-N7A-C5A	2.03	109.87	103.58
3	A	901	NAP	O3D-C3D-C4D	2.02	117.02	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	NAP	O5B-PA-O1A	-2.01	101.50	109.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	485/513 (94%)	-0.28	3 (0%) 86 89	26, 50, 70, 84	0
1	B	484/513 (94%)	-0.47	2 (0%) 90 91	28, 44, 63, 87	0
1	C	485/513 (94%)	-0.24	8 (1%) 68 69	34, 53, 74, 94	0
1	D	484/513 (94%)	-0.34	7 (1%) 72 72	28, 49, 70, 89	0
All	All	1938/2052 (94%)	-0.33	20 (1%) 79 81	26, 49, 71, 94	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	493	LEU	5.3
1	D	92	GLU	3.7
1	C	275	ASN	2.9
1	D	93	THR	2.8
1	C	493	LEU	2.7
1	C	10	SER	2.5
1	C	146	LYS	2.5
1	D	430	LYS	2.4
1	C	151	ILE	2.4
1	B	490	ALA	2.3
1	D	312	LYS	2.2
1	D	91	GLU	2.2
1	A	312	LYS	2.2
1	B	277	GLU	2.2
1	D	279	ILE	2.2
1	C	148	LYS	2.2
1	A	148	LYS	2.1
1	C	397	GLU	2.1
1	A	158	LEU	2.1
1	C	52	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FAD	A	900	53/53	0.17	0.30	42,50,68,68	0
2	FAD	C	900	53/53	0.16	0.27	38,48,65,66	0
2	FAD	B	900	53/53	0.13	0.11	30,37,43,43	0
2	FAD	D	900	53/53	0.13	-0.25	30,42,49,51	0
3	NAP	D	901	48/48	0.13	-0.35	51,60,83,85	0
3	NAP	B	901	48/48	0.12	-0.45	45,53,63,64	0
3	NAP	C	901	48/48	0.14	-0.64	61,72,86,87	0
3	NAP	A	901	48/48	0.14	-0.67	49,64,87,87	0

6.5 Other polymers ⓘ

There are no such residues in this entry.