Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 08:49 AM EDT

PDB ID	:	2R2N
Title	:	The crystal structure of human kynurenine aminotransferase II in complex with kynurenine
Authors	:	Han, Q.; Robinson, H.; Li, J.
Deposited on	:	2007-08-27
Resolution	:	1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

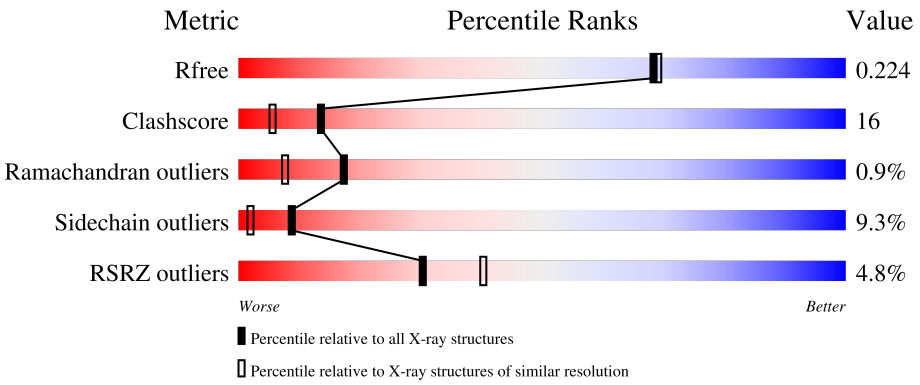
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	425	6% 69% 23% 7% •
1	B	425	5% 69% 25% 5%
1	C	425	4% 70% 25% 5%
1	D	425	4% 75% 20% •

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	429	-	-	X	-
4	GOL	C	429	-	-	X	-
4	GOL	D	427	-	-	X	-
4	GOL	D	429	-	-	X	-

2 Entry composition (i)

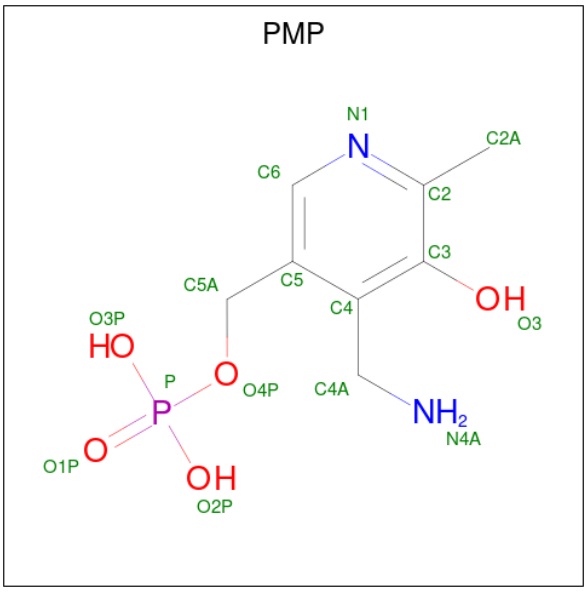
There are 5 unique types of molecules in this entry. The entry contains 14831 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Kynurenine/alpha-aminoadipate aminotransferase mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	425	3332	2139	559	616	18	0	0	0
1	B	425	3333	2139	559	617	18	0	0	0
1	C	425	3332	2139	559	616	18	0	0	0
1	D	425	3333	2139	559	617	18	0	0	0

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	16	8	2	5	1	0	0

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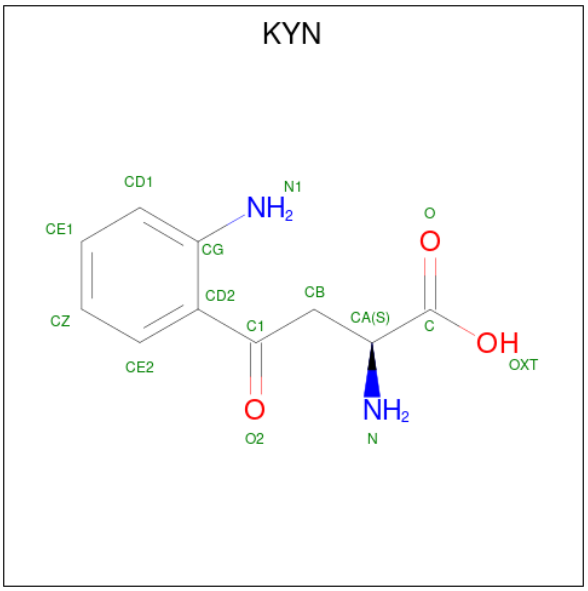
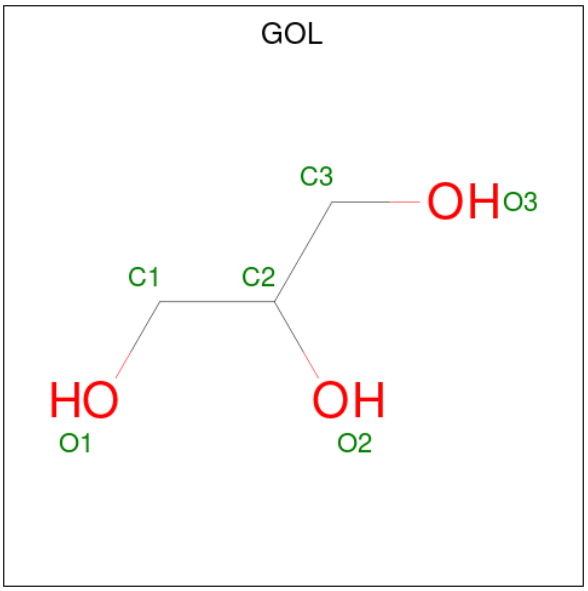
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	16	8	2	5	1	0	0
			Total	C	N	O	P		
2	C	1	16	8	2	5	1	0	0
			Total	C	N	O	P		
2	D	1	16	8	2	5	1	0	0

- Molecule 3 is (2S)-2-amino-4-(2-aminophenyl)-4-oxobutanoic acid (three-letter code: KYN) (formula: $C_{10}H_{12}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	15	10	2	3	0	0
			Total	C	N	O		
3	A	1	15	10	2	3	0	0
			Total	C	N	O		
3	C	1	15	10	2	3	0	0
			Total	C	N	O		
3	C	1	15	10	2	3	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	C	1	6	3	3	0	0
			Total	C	O		
4	D	1	6	3	3	0	0
			Total	C	O		
4	D	1	6	3	3	0	0
			Total	C	O		
4	D	1	6	3	3	0	0
			Total	C	O		
4	D	1	6	3	3	0	0

- Molecule 5 is water.

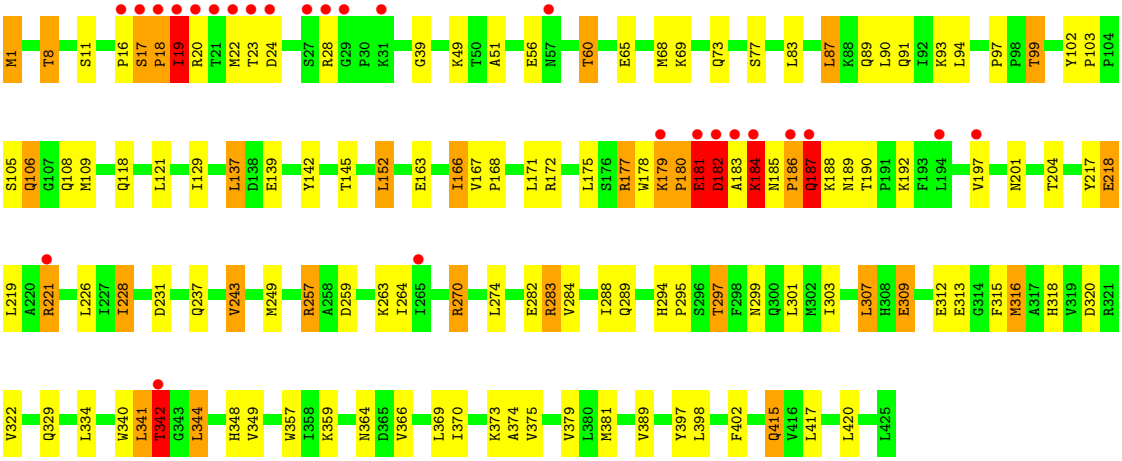
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	314	314	314	0	0
			Total	O		
5	B	325	325	325	0	0
			Total	O		
5	C	352	352	352	0	0
			Total	O		
5	D	350	350	350	0	0

3 Residue-property plots (i)

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

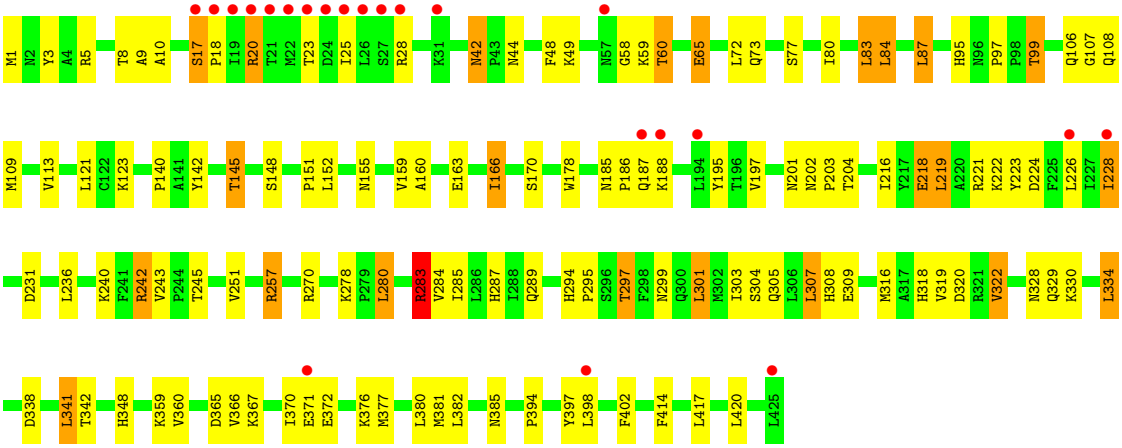
• Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial

Chain A:



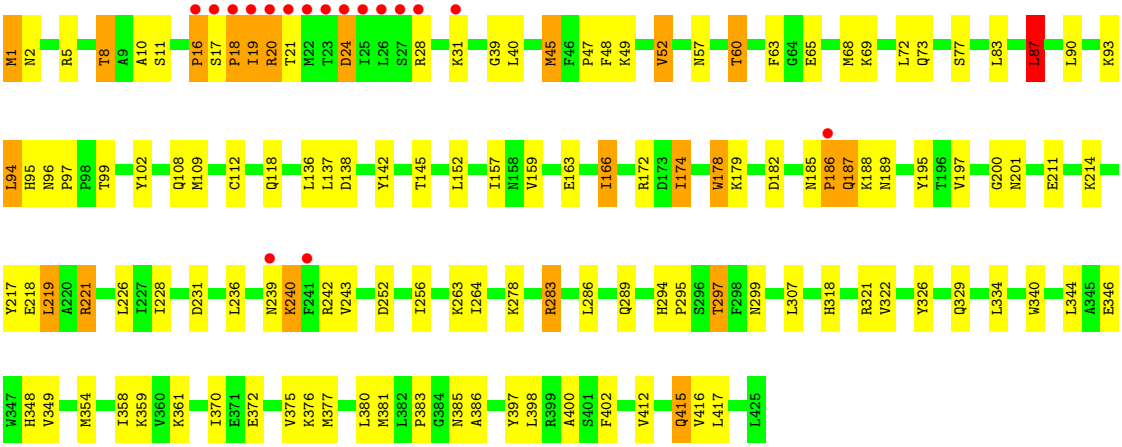
• Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial

Chain B:



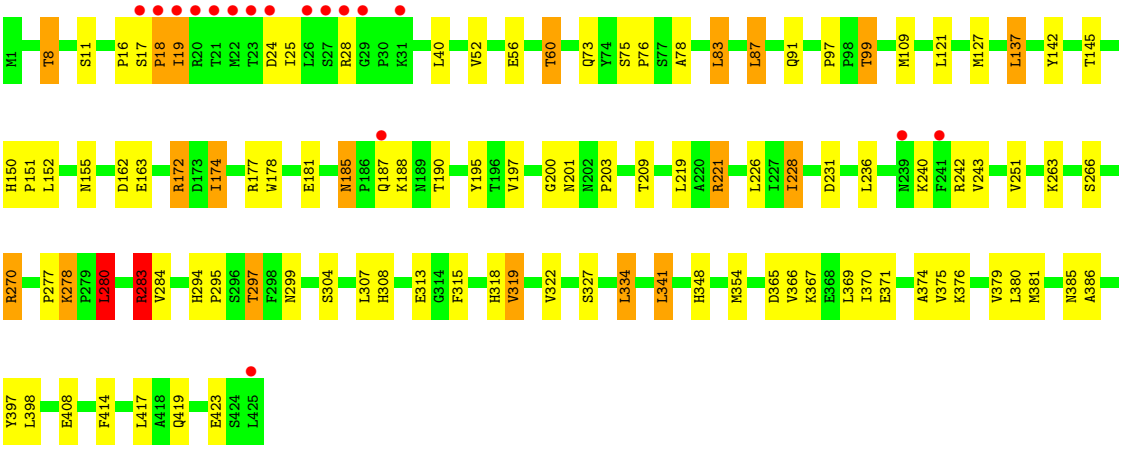
• Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial

Chain C:



- Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.84Å 109.36Å 119.35Å 90.00° 94.68° 90.00°	Depositor
Resolution (Å)	26.68 – 1.95 26.67 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.1 (26.68-1.95) 93.1 (26.67-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.194 , 0.223 0.194 , 0.224	Depositor DCC
R_{free} test set	6185 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14831	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3905e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PMP, KYN

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	0.76	0/3414	0.85	5/4634 (0.1%)
1	B	0.77	0/3415	0.88	6/4634 (0.1%)
1	C	0.84	1/3414 (0.0%)	0.91	8/4634 (0.2%)
1	D	0.87	0/3415	0.94	9/4634 (0.2%)
All	All	0.81	1/13658 (0.0%)	0.89	28/18536 (0.2%)

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	A	0	5
1	C	0	3
1	D	0	2
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	112	CYS	CB-SG	-5.07	1.73	1.81

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	283	ARG	NE-CZ-NH1	13.52	127.06	120.30
1	B	257	ARG	NE-CZ-NH2	-12.38	114.11	120.30
1	A	257	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	B	257	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	C	321	ARG	NE-CZ-NH2	-11.26	114.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	283	ARG	NE-CZ-NH2	-11.23	114.68	120.30
1	A	257	ARG	NE-CZ-NH1	11.21	125.90	120.30
1	C	283	ARG	NE-CZ-NH2	-10.96	114.82	120.30
1	D	242	ARG	NE-CZ-NH2	-10.84	114.88	120.30
1	C	321	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	D	242	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	C	283	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	B	283	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	B	242	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	A	283	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	D	231	ASP	CB-CG-OD1	6.55	124.20	118.30
1	C	45	MET	CG-SD-CE	5.77	109.43	100.20
1	B	283	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	231	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	242	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	280	LEU	CB-CG-CD1	5.55	120.44	111.00
1	D	270	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	87	LEU	CB-CG-CD1	5.39	120.16	111.00
1	A	182	ASP	CB-CG-OD2	5.38	123.15	118.30
1	D	172	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	270	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	D	334	LEU	CB-CG-CD1	5.28	119.98	111.00
1	C	242	ARG	NE-CZ-NH2	-5.25	117.67	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	PRO	Peptide
1	A	181	GLU	Peptide
1	A	187	GLN	Peptide
1	A	341	LEU	Peptide
1	A	342	THR	Peptide
1	C	16	PRO	Peptide
1	C	187	GLN	Peptide
1	C	240	LYS	Peptide
1	D	16	PRO	Peptide
1	D	240	LYS	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	3332	0	3353	131	0
1	B	3333	0	3353	105	0
1	C	3332	0	3353	109	0
1	D	3333	0	3353	94	0
2	A	16	0	11	3	0
2	B	16	0	11	2	0
2	C	16	0	11	2	0
2	D	16	0	11	4	0
3	A	30	0	23	4	0
3	C	30	0	22	5	0
4	A	6	0	7	6	0
4	C	6	0	8	6	0
4	D	24	0	32	12	0
5	A	314	0	0	20	0
5	B	325	0	0	17	0
5	C	352	0	0	19	0
5	D	350	0	0	12	0
All	All	14831	0	13548	433	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 16.

All (433) 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:B:17:SER:HB2	1:B:18:PRO:HA	1.23	1.17
1:C:370:ILE:HD11	1:C:398:LEU:CD2	1.76	1.14
1:C:370:ILE:HD11	1:C:398:LEU:HD21	1.15	1.09
1:D:381:MET:HE2	1:D:398:LEU:HD13	1.34	1.05
1:D:78:ALA:HB3	4:D:427:GOL:H12	1.34	1.04
1:A:179:LYS:O	1:A:182:ASP:HB2	1.56	1.04
1:A:69:LYS:HG2	4:A:429:GOL:H2	1.36	1.01
1:C:45:MET:HE2	1:D:322:VAL:HG22	1.43	1.01
1:B:17:SER:HB2	1:B:18:PRO:CA	1.94	0.97
1:B:20:ARG:HG2	1:B:20:ARG:HH11	1.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ILE:HG13	1:B:398:LEU:HD21	1.47	0.96
1:D:17:SER:HB3	1:D:18:PRO:HA	1.46	0.96
1:A:182:ASP:HA	1:A:188:LYS:HD2	1.54	0.89
1:A:142:TYR:O	1:A:145:THR:HG22	1.72	0.89
1:A:19:ILE:HG22	1:A:20:ARG:N	1.85	0.89
1:A:179:LYS:HG3	1:A:181:GLU:OE1	1.73	0.89
1:D:8:THR:HG21	5:D:478:HOH:O	1.75	0.87
1:A:179:LYS:O	1:A:182:ASP:CB	2.23	0.86
1:D:381:MET:CE	1:D:398:LEU:HD13	2.06	0.84
1:A:184:LYS:HD3	5:A:664:HOH:O	1.77	0.84
1:A:69:LYS:CG	4:A:429:GOL:H2	2.09	0.82
1:C:370:ILE:CD1	1:C:398:LEU:HD21	2.07	0.81
1:C:381:MET:CE	1:C:400:ALA:HB2	2.10	0.81
1:A:182:ASP:HA	1:A:188:LYS:CD	2.10	0.81
1:A:184:LYS:H	1:A:184:LYS:HD2	1.46	0.81
1:D:145:THR:HG21	1:D:195:TYR:OH	1.81	0.80
1:C:99:THR:HG21	5:C:437:HOH:O	1.83	0.79
1:C:283:ARG:HD3	5:C:511:HOH:O	1.81	0.79
4:D:429:GOL:H11	5:D:759:HOH:O	1.83	0.79
1:A:65:GLU:HG2	5:A:577:HOH:O	1.83	0.78
1:C:17:SER:HB3	1:C:18:PRO:HA	1.63	0.78
4:A:429:GOL:H11	5:A:532:HOH:O	1.82	0.77
1:D:318:HIS:ND1	4:D:429:GOL:H32	1.98	0.77
1:B:367:LYS:O	1:B:371:GLU:HG2	1.86	0.74
1:B:83:LEU:HD22	1:B:87:LEU:HD22	1.69	0.74
1:A:366:VAL:HG23	1:A:369:LEU:HD23	1.70	0.74
1:D:99:THR:HG21	5:D:706:HOH:O	1.87	0.74
1:C:381:MET:HE1	1:C:400:ALA:HB2	1.67	0.74
1:D:8:THR:HG22	1:D:11:SER:H	1.52	0.73
1:A:183:ALA:C	1:A:185:ASN:H	1.93	0.72
1:A:221:ARG:HD2	5:A:584:HOH:O	1.87	0.72
1:D:76:PRO:HB3	4:D:427:GOL:H2	1.71	0.72
1:A:370:ILE:HG13	1:A:398:LEU:HD21	1.71	0.71
1:C:294:HIS:HD2	1:C:295:PRO:O	1.73	0.71
1:D:197:VAL:HB	1:D:201:ASN:HD22	1.56	0.71
1:B:320:ASP:HB3	5:B:672:HOH:O	1.91	0.70
1:C:8:THR:HG22	1:C:11:SER:H	1.55	0.70
1:C:263:LYS:HZ3	2:C:426:PMP:H4A1	1.55	0.70
1:A:8:THR:HG21	5:A:434:HOH:O	1.92	0.70
1:C:142:TYR:HD1	1:C:145:THR:HG23	1.56	0.70
1:A:19:ILE:HG13	1:B:382:LEU:HD21	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:VAL:HG12	5:C:541:HOH:O	1.92	0.69
1:D:17:SER:HB3	1:D:18:PRO:CA	2.20	0.69
1:C:73:GLN:O	1:C:297:THR:HG21	1.92	0.69
1:D:367:LYS:O	1:D:371:GLU:HG2	1.93	0.69
1:A:294:HIS:HD2	1:A:295:PRO:O	1.75	0.69
1:A:19:ILE:CG2	1:A:20:ARG:N	2.55	0.69
1:A:166:ILE:HG21	5:A:679:HOH:O	1.92	0.69
1:C:90:LEU:HG	1:C:94:LEU:HD22	1.75	0.68
1:B:178:TRP:CZ3	1:B:188:LYS:O	2.46	0.68
1:C:60:THR:HG22	5:C:459:HOH:O	1.93	0.68
1:A:179:LYS:CG	1:A:181:GLU:OE1	2.40	0.68
1:D:209:THR:HG22	4:D:430:GOL:H2	1.76	0.68
1:B:142:TYR:CD2	1:B:145:THR:HG22	2.28	0.68
1:A:49:LYS:HA	4:A:429:GOL:H12	1.74	0.68
1:A:342:THR:H	1:A:344:LEU:H	1.40	0.67
1:C:19:ILE:HG23	5:C:708:HOH:O	1.95	0.67
1:B:338:ASP:O	1:B:342:THR:HG23	1.93	0.67
1:C:370:ILE:CD1	1:C:398:LEU:CD2	2.65	0.67
1:B:20:ARG:HH11	1:B:20:ARG:CG	2.06	0.67
1:C:145:THR:HG21	1:C:195:TYR:OH	1.95	0.67
2:D:426:PMP:O3	2:D:426:PMP:N4A	2.28	0.67
1:A:8:THR:CG2	1:A:11:SER:H	2.09	0.66
1:B:99:THR:HG21	5:B:511:HOH:O	1.95	0.66
1:A:73:GLN:O	1:A:297:THR:HG21	1.95	0.66
1:A:163:GLU:HG3	1:A:348:HIS:CE1	2.31	0.66
1:B:370:ILE:CG1	1:B:398:LEU:HD21	2.25	0.66
1:C:385:ASN:HB2	5:C:649:HOH:O	1.95	0.66
1:B:178:TRP:HZ3	1:B:188:LYS:O	1.79	0.66
1:A:182:ASP:HA	1:A:188:LYS:CE	2.26	0.65
1:A:197:VAL:HB	1:A:201:ASN:HD22	1.61	0.65
1:B:5:ARG:NH2	1:B:224:ASP:OD2	2.29	0.65
1:D:145:THR:HG22	5:D:680:HOH:O	1.96	0.65
1:A:349:VAL:HG12	5:A:579:HOH:O	1.96	0.65
1:C:186:PRO:O	1:C:187:GLN:HG2	1.96	0.65
1:D:145:THR:HG21	1:D:195:TYR:CZ	2.31	0.64
1:B:42:ASN:HD22	1:B:44:ASN:H	1.45	0.64
1:D:76:PRO:CB	4:D:427:GOL:H2	2.28	0.64
1:A:217:TYR:HB2	1:A:249:MET:HE3	1.80	0.64
1:C:145:THR:HG21	1:C:195:TYR:CZ	2.33	0.64
4:C:429:GOL:H2	5:C:702:HOH:O	1.98	0.63
1:C:263:LYS:NZ	2:C:426:PMP:H4A1	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:GLU:HG3	1:D:348:HIS:CE1	2.33	0.63
1:A:263:LYS:NZ	2:A:426:PMP:H4A2	2.12	0.63
1:A:217:TYR:HB2	1:A:249:MET:CE	2.29	0.63
3:C:427:KYN:H	2:D:426:PMP:HNA2	1.47	0.63
1:A:20:ARG:HG2	1:A:23:THR:OG1	1.98	0.62
1:D:60:THR:HG22	5:D:705:HOH:O	1.99	0.62
1:A:49:LYS:HD2	4:A:429:GOL:H12	1.80	0.62
1:A:263:LYS:HZ3	2:A:426:PMP:H4A2	1.64	0.62
1:D:283:ARG:HD3	5:D:510:HOH:O	1.99	0.62
1:C:17:SER:HB3	1:C:18:PRO:CA	2.29	0.62
1:B:163:GLU:HG3	1:B:348:HIS:CE1	2.35	0.62
1:D:8:THR:CG2	1:D:11:SER:H	2.12	0.62
1:A:137:LEU:C	1:A:137:LEU:HD23	2.21	0.61
3:C:428:KYN:OXT	1:D:19:ILE:HG12	2.00	0.61
1:D:263:LYS:NZ	2:D:426:PMP:H4A2	2.15	0.61
1:A:60:THR:HG22	5:A:734:HOH:O	1.99	0.61
1:A:299:ASN:HD21	1:B:299:ASN:HD21	1.47	0.61
1:D:263:LYS:HZ1	2:D:426:PMP:H4A2	1.65	0.61
1:B:142:TYR:HD2	1:B:145:THR:HG22	1.66	0.60
1:B:60:THR:HG22	5:B:457:HOH:O	2.02	0.60
1:B:148:SER:O	1:B:152:LEU:HD23	2.01	0.60
1:D:294:HIS:HD2	1:D:295:PRO:O	1.85	0.60
1:A:103:PRO:HB2	1:A:106:GLN:HG3	1.84	0.60
1:D:73:GLN:O	1:D:297:THR:HG21	2.01	0.60
1:A:8:THR:HG22	1:A:11:SER:H	1.64	0.59
1:A:56:GLU:HA	5:A:618:HOH:O	2.01	0.59
1:B:365:ASP:HB2	1:B:394:PRO:HB3	1.84	0.59
1:C:178:TRP:CZ3	1:C:188:LYS:O	2.56	0.59
1:A:179:LYS:O	1:A:182:ASP:CG	2.41	0.58
1:C:359:LYS:HB2	1:C:397:TYR:CE2	2.38	0.58
1:A:180:PRO:O	1:A:183:ALA:N	2.36	0.58
1:C:99:THR:HG23	1:C:109:MET:HB2	1.86	0.58
1:D:142:TYR:HD2	1:D:145:THR:HG23	1.69	0.58
1:C:19:ILE:HD12	1:C:19:ILE:H	1.67	0.58
1:C:346:GLU:HG3	1:C:361:LYS:HE3	1.85	0.58
1:A:163:GLU:CG	1:A:348:HIS:CE1	2.86	0.58
1:A:183:ALA:C	1:A:185:ASN:N	2.57	0.58
1:B:294:HIS:HD2	1:B:295:PRO:O	1.86	0.58
1:D:397:TYR:HE1	4:D:428:GOL:H32	1.69	0.58
1:C:372:GLU:HG2	5:C:698:HOH:O	2.04	0.57
1:C:386:ALA:HB1	1:D:18:PRO:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLN:O	1:B:297:THR:HG21	2.03	0.57
1:B:106:GLN:NE2	5:B:530:HOH:O	2.36	0.57
1:C:381:MET:HE3	1:C:400:ALA:HB2	1.85	0.57
1:C:370:ILE:HD11	1:C:398:LEU:HD23	1.78	0.57
1:D:370:ILE:HG21	1:D:381:MET:O	2.05	0.57
1:B:77:SER:OG	1:B:289:GLN:HG2	2.04	0.57
1:B:84:LEU:HD13	1:B:113:VAL:HG23	1.85	0.56
1:B:381:MET:HE2	1:B:398:LEU:HD13	1.86	0.56
1:D:163:GLU:CG	1:D:348:HIS:CE1	2.88	0.56
1:D:385:ASN:ND2	5:D:700:HOH:O	2.38	0.56
1:D:348:HIS:CD2	4:D:428:GOL:H2	2.40	0.56
1:A:182:ASP:CA	1:A:188:LYS:HD2	2.34	0.56
1:A:231:ASP:OD2	1:A:257:ARG:NH2	2.37	0.56
1:B:377:MET:HG3	1:B:420:LEU:HD11	1.87	0.56
1:C:142:TYR:CD1	1:C:145:THR:HG23	2.38	0.56
1:A:381:MET:HE2	1:A:398:LEU:HD13	1.88	0.56
1:B:121:LEU:CD2	1:B:228:ILE:HD11	2.35	0.56
1:C:136:LEU:HD21	1:C:174:ILE:HD11	1.87	0.56
1:C:264:ILE:O	1:C:318:HIS:HE1	1.89	0.56
1:C:386:ALA:HB1	1:D:18:PRO:CG	2.36	0.55
1:D:78:ALA:CB	4:D:427:GOL:H12	2.22	0.55
1:C:2:ASN:O	1:C:5:ARG:HG2	2.06	0.55
1:C:97:PRO:HG2	1:C:109:MET:SD	2.46	0.55
1:C:60:THR:HG23	5:C:505:HOH:O	2.05	0.55
1:B:341:LEU:HD22	1:B:414:PHE:HD2	1.71	0.55
1:B:159:VAL:HG11	1:B:166:ILE:HD12	1.88	0.55
1:C:18:PRO:HG2	1:D:386:ALA:HB1	1.88	0.55
1:A:172:ARG:NH2	1:A:218:GLU:OE1	2.40	0.55
1:C:95:HIS:HE1	5:C:463:HOH:O	1.88	0.55
4:C:429:GOL:C2	5:C:702:HOH:O	2.55	0.55
1:C:57:ASN:HD22	4:C:429:GOL:H31	1.72	0.55
1:A:93:LYS:HG3	1:A:312:GLU:OE2	2.07	0.55
1:A:294:HIS:CE1	1:B:270:ARG:HD3	2.42	0.55
1:A:99:THR:HG21	5:A:513:HOH:O	2.06	0.54
1:B:20:ARG:HB3	1:B:23:THR:HG22	1.90	0.54
1:C:47:PRO:HB3	4:D:429:GOL:H31	1.87	0.54
1:C:83:LEU:HG	1:C:87:LEU:HD22	1.88	0.54
1:C:178:TRP:HZ3	1:C:188:LYS:O	1.89	0.54
1:B:80:ILE:HD13	1:B:301:LEU:HD13	1.89	0.54
1:C:8:THR:HG21	5:C:512:HOH:O	2.08	0.54
1:A:179:LYS:CD	1:A:181:GLU:OE1	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ASP:OD2	1:B:257:ARG:NH2	2.40	0.53
1:B:370:ILE:HG13	1:B:398:LEU:CD2	2.29	0.53
1:A:166:ILE:CG2	5:A:679:HOH:O	2.54	0.53
1:D:163:GLU:HG3	1:D:348:HIS:NE2	2.24	0.53
1:D:172:ARG:NH2	5:D:507:HOH:O	2.40	0.53
1:C:163:GLU:HG2	1:C:348:HIS:CE1	2.44	0.53
1:A:340:TRP:CE2	1:A:415:GLN:HB3	2.44	0.53
1:D:185:ASN:ND2	1:D:187:GLN:H	2.07	0.53
1:A:175:LEU:HD12	1:A:219:LEU:HD22	1.91	0.53
1:C:45:MET:HE2	1:D:322:VAL:CG2	2.28	0.53
3:C:428:KYN:HZ	1:D:40:LEU:HD21	1.89	0.53
1:D:375:VAL:HG12	1:D:380:LEU:CD2	2.39	0.53
1:D:19:ILE:HD12	1:D:19:ILE:H	1.73	0.52
1:C:16:PRO:HA	1:C:286:LEU:HD21	1.92	0.52
1:C:349:VAL:HG13	5:C:462:HOH:O	2.07	0.52
1:D:304:SER:O	1:D:308:HIS:HD2	1.93	0.52
1:D:366:VAL:CG2	1:D:369:LEU:HD23	2.40	0.52
1:C:138:ASP:HB3	1:C:166:ILE:HG22	1.91	0.52
1:B:145:THR:HG21	1:B:195:TYR:OH	2.09	0.52
2:B:426:PMP:O3	2:B:426:PMP:N4A	2.42	0.52
1:C:39:GLY:HA3	3:C:427:KYN:HA	1.91	0.52
1:C:185:ASN:O	1:C:186:PRO:C	2.48	0.52
1:B:316:MET:HA	1:B:319:VAL:HG13	1.91	0.52
1:D:142:TYR:CD2	1:D:145:THR:HG23	2.45	0.52
1:D:142:TYR:HB2	5:D:676:HOH:O	2.10	0.52
1:B:121:LEU:HD22	1:B:228:ILE:HD11	1.92	0.52
2:A:426:PMP:O3	2:A:426:PMP:N4A	2.41	0.51
1:A:102:TYR:O	1:A:108:GLN:HB2	2.09	0.51
1:A:263:LYS:N	1:A:263:LYS:HD2	2.25	0.51
1:B:17:SER:CB	1:B:18:PRO:CA	2.77	0.51
1:C:187:GLN:C	1:C:189:ASN:H	2.14	0.51
1:A:8:THR:HG22	1:A:11:SER:HB3	1.91	0.51
1:A:24:ASP:HB2	5:A:658:HOH:O	2.10	0.51
1:A:137:LEU:C	1:A:137:LEU:CD2	2.79	0.51
3:A:427:KYN:H	1:B:202:ASN:HD21	1.59	0.51
1:B:381:MET:CE	1:B:398:LEU:HD13	2.40	0.51
1:C:375:VAL:HG12	1:C:380:LEU:HD21	1.91	0.51
3:A:427:KYN:HD1	5:A:515:HOH:O	2.11	0.51
1:B:341:LEU:HD22	1:B:414:PHE:CD2	2.45	0.51
1:D:397:TYR:CE1	4:D:428:GOL:H32	2.46	0.51
1:D:419:GLN:HE21	1:D:423:GLU:HG3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:429:GOL:C3	5:C:702:HOH:O	2.58	0.51
1:C:377:MET:HE3	5:C:682:HOH:O	2.09	0.50
1:A:237:GLN:HE22	1:A:243:VAL:H	1.59	0.50
1:A:19:ILE:CG1	1:B:382:LEU:HD21	2.42	0.50
4:C:429:GOL:H32	5:C:702:HOH:O	2.11	0.50
1:A:139:GLU:OE1	1:A:389:VAL:HG23	2.11	0.50
1:A:342:THR:N	1:A:344:LEU:H	2.09	0.50
1:B:3:TYR:CD2	1:B:280:LEU:HD21	2.47	0.50
1:B:318:HIS:O	1:B:322:VAL:HG12	2.12	0.50
1:D:87:LEU:O	1:D:91:GLN:HG2	2.12	0.50
1:D:150:HIS:HB3	1:D:151:PRO:HD3	1.93	0.50
1:D:366:VAL:HG23	1:D:369:LEU:HD23	1.93	0.50
1:B:80:ILE:CD1	1:B:301:LEU:HD13	2.42	0.50
1:B:359:LYS:HB2	1:B:397:TYR:CE1	2.47	0.50
1:C:48:PHE:HB2	1:C:72:LEU:HD11	1.94	0.50
1:A:315:PHE:HD2	1:A:316:MET:CE	2.25	0.50
1:A:381:MET:CE	1:A:398:LEU:HB3	2.42	0.49
1:B:218:GLU:HG2	1:B:219:LEU:N	2.26	0.49
1:C:221:ARG:HG2	1:C:252:ASP:OD2	2.11	0.49
1:A:18:PRO:O	1:A:20:ARG:N	2.45	0.49
1:A:97:PRO:HG2	1:A:109:MET:SD	2.52	0.49
1:C:8:THR:CG2	1:C:11:SER:H	2.25	0.49
1:D:185:ASN:C	1:D:185:ASN:HD22	2.14	0.49
1:A:179:LYS:HD3	1:A:181:GLU:OE1	2.11	0.49
1:A:182:ASP:O	1:A:185:ASN:O	2.30	0.49
1:A:283:ARG:HD3	5:A:729:HOH:O	2.12	0.49
1:C:157:ILE:HG21	1:C:174:ILE:HD13	1.94	0.49
1:B:366:VAL:HG22	1:B:370:ILE:HG12	1.94	0.49
1:C:370:ILE:CD1	1:C:383:PRO:HG3	2.43	0.49
1:D:221:ARG:HH22	1:D:251:VAL:CG1	2.25	0.49
1:D:408:GLU:CD	1:D:408:GLU:H	2.14	0.49
1:A:270:ARG:HD3	1:B:294:HIS:CE1	2.48	0.49
1:B:303:ILE:HG22	1:B:307:LEU:HD22	1.95	0.49
1:C:73:GLN:O	1:C:297:THR:CG2	2.59	0.49
1:B:42:ASN:ND2	1:B:44:ASN:H	2.09	0.49
1:C:16:PRO:HD3	5:C:733:HOH:O	2.13	0.49
1:C:197:VAL:HB	1:C:201:ASN:HD22	1.77	0.49
1:C:370:ILE:HD13	1:C:383:PRO:HG3	1.94	0.49
1:B:42:ASN:ND2	1:B:44:ASN:HB2	2.28	0.48
1:A:8:THR:HG22	1:A:11:SER:CB	2.43	0.48
1:A:171:LEU:HG	1:A:219:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LYS:HG2	1:B:334:LEU:HD22	1.94	0.48
1:C:375:VAL:HG12	1:C:380:LEU:CD2	2.44	0.48
1:B:188:LYS:HB2	5:B:740:HOH:O	2.14	0.48
1:A:179:LYS:N	1:A:182:ASP:OD2	2.40	0.48
1:C:45:MET:CE	1:D:322:VAL:HA	2.44	0.48
1:C:195:TYR:HA	1:C:228:ILE:HG23	1.96	0.48
1:C:221:ARG:HH11	1:C:221:ARG:HB3	1.77	0.48
1:A:90:LEU:HG	1:A:94:LEU:HD22	1.96	0.48
1:D:381:MET:CE	1:D:398:LEU:CD1	2.87	0.48
1:A:370:ILE:HG23	5:A:737:HOH:O	2.12	0.47
1:C:16:PRO:HA	1:C:286:LEU:CD2	2.44	0.47
1:C:52:VAL:HG13	1:D:52:VAL:HB	1.96	0.47
1:A:177:ARG:HH11	1:A:177:ARG:HB2	1.79	0.47
1:A:121:LEU:HD23	1:A:228:ILE:HD11	1.95	0.47
1:A:299:ASN:ND2	1:B:299:ASN:HD21	2.12	0.47
1:C:412:VAL:O	1:C:415:GLN:HG3	2.14	0.47
1:D:283:ARG:N	1:D:283:ARG:HD2	2.30	0.47
1:D:178:TRP:CD1	1:D:190:THR:HG22	2.49	0.47
1:A:370:ILE:HG13	1:A:398:LEU:CD2	2.43	0.47
1:B:160:ALA:HB3	1:B:170:SER:CB	2.45	0.47
1:A:373:LYS:HB3	1:A:420:LEU:HD22	1.96	0.47
1:A:370:ILE:CG1	1:A:398:LEU:HD21	2.42	0.46
1:B:20:ARG:CG	1:B:20:ARG:NH1	2.72	0.46
1:B:42:ASN:HD21	1:B:44:ASN:HB2	1.81	0.46
1:C:299:ASN:HD21	1:D:299:ASN:HD21	1.64	0.46
1:A:121:LEU:CD2	1:A:228:ILE:HD11	2.46	0.46
1:D:8:THR:HG22	1:D:11:SER:CB	2.45	0.46
1:D:221:ARG:HH22	1:D:251:VAL:HG11	1.80	0.46
1:D:354:MET:HB3	1:D:354:MET:HE2	1.80	0.46
1:A:142:TYR:O	1:A:145:THR:CG2	2.55	0.46
1:A:366:VAL:HG22	1:A:370:ILE:HG12	1.98	0.46
1:B:20:ARG:HG2	1:B:20:ARG:NH1	2.07	0.46
1:B:372:GLU:O	1:B:376:LYS:HE2	2.16	0.46
1:C:77:SER:OG	1:C:289:GLN:HG2	2.16	0.46
1:C:63:PHE:HD2	1:C:68:MET:HE1	1.80	0.46
1:D:375:VAL:HG12	1:D:380:LEU:HD22	1.96	0.46
1:A:349:VAL:HG13	5:A:488:HOH:O	2.16	0.46
1:B:380:LEU:HA	5:B:664:HOH:O	2.16	0.46
1:B:366:VAL:HG12	5:B:697:HOH:O	2.16	0.46
1:A:19:ILE:HG22	1:A:20:ARG:HG3	1.98	0.46
1:D:185:ASN:HD21	1:D:187:GLN:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:MET:CE	1:A:398:LEU:HD13	2.46	0.46
3:A:427:KYN:O2	2:B:426:PMP:H4A1	2.15	0.46
1:B:305:GLN:NE2	5:B:557:HOH:O	2.48	0.46
1:D:163:GLU:H	1:D:163:GLU:CD	2.18	0.45
1:A:274:LEU:HD23	1:A:284:VAL:HG21	1.98	0.45
1:B:197:VAL:HB	1:B:201:ASN:HD22	1.81	0.45
1:B:142:TYR:HB2	5:B:665:HOH:O	2.16	0.45
1:D:155:ASN:HB3	5:D:643:HOH:O	2.17	0.45
1:B:329:GLN:HB3	1:B:402:PHE:O	2.16	0.45
1:B:1:MET:HG2	5:B:732:HOH:O	2.16	0.45
1:C:21:THR:HA	1:C:24:ASP:HB3	1.99	0.45
1:D:8:THR:HB	1:D:127:MET:O	2.16	0.45
4:D:429:GOL:C1	5:D:759:HOH:O	2.56	0.45
1:B:17:SER:CB	1:B:18:PRO:HA	2.16	0.45
1:B:148:SER:O	1:B:151:PRO:HD2	2.17	0.45
1:A:73:GLN:O	1:A:297:THR:CG2	2.64	0.45
1:A:309:GLU:OE1	1:D:188:LYS:NZ	2.38	0.45
1:C:159:VAL:HG11	1:C:166:ILE:HD13	1.98	0.45
1:A:282:GLU:OE2	1:A:283:ARG:NH1	2.50	0.45
1:B:25:ILE:HD12	1:B:28:ARG:NH2	2.32	0.45
1:C:19:ILE:HG22	1:C:20:ARG:N	2.32	0.45
1:C:163:GLU:CG	1:C:348:HIS:CE1	2.99	0.45
1:A:283:ARG:N	1:A:283:ARG:HD2	2.32	0.45
1:B:8:THR:CG2	1:B:9:ALA:N	2.80	0.44
1:C:172:ARG:HG3	1:C:219:LEU:HD11	1.99	0.44
1:B:65:GLU:H	1:B:65:GLU:HG2	1.63	0.44
1:D:365:ASP:OD1	1:D:367:LYS:HB2	2.17	0.44
1:D:174:ILE:C	1:D:174:ILE:HD12	2.37	0.44
1:B:8:THR:HG22	1:B:10:ALA:N	2.33	0.44
1:C:182:ASP:HB3	1:C:188:LYS:HB2	2.00	0.44
1:A:105:SER:O	5:A:595:HOH:O	2.21	0.44
1:A:204:THR:HA	1:A:357:TRP:HB2	2.00	0.44
1:A:257:ARG:HD3	1:A:259:ASP:OD2	2.18	0.44
1:B:123:LYS:HD3	1:B:287:HIS:HB3	1.99	0.44
1:D:75:SER:HB2	1:D:76:PRO:CD	2.48	0.44
1:C:294:HIS:NE2	1:D:270:ARG:HD3	2.33	0.44
1:C:217:TYR:O	1:C:221:ARG:HG3	2.18	0.43
1:A:89:GLN:OE1	1:A:93:LYS:HE3	2.18	0.43
1:B:166:ILE:HG12	1:B:216:ILE:HD11	2.00	0.43
1:C:200:GLY:O	1:C:201:ASN:C	2.56	0.43
1:A:91:GLN:HA	1:A:91:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LYS:H	1:A:184:LYS:CD	2.25	0.43
1:C:240:LYS:HA	5:C:630:HOH:O	2.16	0.43
1:D:315:PHE:O	1:D:319:VAL:HG13	2.18	0.43
1:A:303:ILE:HG22	1:A:307:LEU:HD22	1.99	0.43
1:A:359:LYS:HB2	1:A:397:TYR:CE2	2.53	0.43
1:A:49:LYS:CD	4:A:429:GOL:H12	2.45	0.43
1:A:264:ILE:O	1:A:318:HIS:HE1	2.00	0.43
1:D:97:PRO:HG2	1:D:109:MET:SD	2.59	0.43
1:D:374:ALA:HB1	1:D:379:VAL:HG23	1.99	0.43
1:A:118:GLN:O	1:A:118:GLN:HG3	2.18	0.43
1:B:163:GLU:CG	1:B:348:HIS:CE1	3.02	0.43
1:C:214:LYS:O	1:C:218:GLU:HG3	2.18	0.43
1:C:358:ILE:HD12	1:C:381:MET:HE1	2.00	0.43
1:A:329:GLN:HB3	1:A:402:PHE:O	2.19	0.43
1:B:371:GLU:HG3	1:B:372:GLU:HG3	2.01	0.43
1:A:77:SER:OG	1:A:289:GLN:HG2	2.18	0.43
1:B:304:SER:O	1:B:308:HIS:HD2	2.01	0.43
1:A:185:ASN:HA	1:A:186:PRO:HD2	1.82	0.43
1:A:370:ILE:O	1:A:375:VAL:HG13	2.19	0.43
1:B:95:HIS:CE1	1:B:245:THR:HG21	2.53	0.43
1:D:370:ILE:HG13	1:D:398:LEU:CD2	2.49	0.43
1:A:381:MET:HE2	1:A:398:LEU:HB3	2.00	0.43
1:B:152:LEU:N	1:B:152:LEU:HD22	2.34	0.43
1:C:182:ASP:HB3	1:C:188:LYS:CB	2.49	0.43
1:C:415:GLN:HG3	1:C:416:VAL:N	2.34	0.43
1:A:374:ALA:HB1	1:A:379:VAL:HG23	2.01	0.42
1:C:1:MET:N	5:C:431:HOH:O	2.35	0.42
1:C:65:GLU:O	1:C:69:LYS:HG3	2.19	0.42
1:C:318:HIS:HD2	4:C:429:GOL:C2	2.32	0.42
1:C:329:GLN:HB3	1:C:402:PHE:O	2.19	0.42
1:B:185:ASN:HA	1:B:186:PRO:HD3	1.90	0.42
1:C:95:HIS:O	1:C:96:ASN:C	2.55	0.42
1:A:270:ARG:HD3	1:B:294:HIS:NE2	2.34	0.42
1:C:340:TRP:CE2	1:C:415:GLN:HB3	2.53	0.42
1:D:121:LEU:HD22	1:D:228:ILE:HD11	2.01	0.42
1:D:162:ASP:HB2	1:D:163:GLU:OE1	2.19	0.42
1:A:178:TRP:CD1	1:A:190:THR:HG22	2.55	0.42
1:A:166:ILE:HG23	5:A:603:HOH:O	2.19	0.42
1:A:342:THR:O	1:A:342:THR:HG23	2.20	0.42
1:B:285:ILE:O	1:B:289:GLN:HG3	2.20	0.42
1:D:83:LEU:HD22	1:D:87:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:GLY:O	1:D:201:ASN:C	2.58	0.42
1:B:222:LYS:HG2	1:B:223:TYR:CE2	2.55	0.42
1:B:398:LEU:HA	1:B:398:LEU:HD23	1.82	0.42
1:A:83:LEU:HG	1:A:87:LEU:HD22	2.00	0.42
1:D:137:LEU:C	1:D:137:LEU:HD23	2.40	0.42
1:A:19:ILE:HG22	1:A:20:ARG:CA	2.47	0.42
1:A:51:ALA:HB2	1:A:68:MET:HE1	2.02	0.41
1:C:40:LEU:CD2	3:C:427:KYN:HZ	2.50	0.41
1:A:181:GLU:C	1:A:183:ALA:N	2.72	0.41
1:B:242:ARG:NH2	1:B:316:MET:CE	2.82	0.41
1:D:185:ASN:HB3	1:D:188:LYS:HG2	2.02	0.41
1:A:181:GLU:C	1:A:183:ALA:H	2.24	0.41
1:B:48:PHE:HB2	1:B:72:LEU:HD11	2.02	0.41
1:B:221:ARG:NH2	1:B:251:VAL:CG1	2.83	0.41
1:C:99:THR:CG2	1:C:109:MET:HB2	2.48	0.41
1:C:102:TYR:O	1:C:108:GLN:HB2	2.19	0.41
1:D:24:ASP:OD2	1:D:25:ILE:N	2.53	0.41
1:A:171:LEU:CG	1:A:219:LEU:HD13	2.50	0.41
1:A:366:VAL:HG22	1:A:366:VAL:O	2.21	0.41
1:B:20:ARG:HB3	1:B:23:THR:CG2	2.51	0.41
1:C:138:ASP:CB	1:C:166:ILE:HG22	2.50	0.41
1:A:342:THR:O	1:A:342:THR:CG2	2.69	0.41
1:D:370:ILE:CG1	1:D:398:LEU:HD21	2.51	0.41
1:B:107:GLY:O	1:B:108:GLN:C	2.58	0.41
1:C:187:GLN:CA	1:C:189:ASN:H	2.33	0.41
1:C:211:GLU:CD	1:C:211:GLU:H	2.24	0.41
1:D:163:GLU:HG2	1:D:348:HIS:CE1	2.55	0.41
1:D:277:PRO:HG2	1:D:280:LEU:HD22	2.03	0.41
1:B:140:PRO:HG2	1:B:204:THR:CG2	2.50	0.41
1:B:160:ALA:HB3	1:B:170:SER:HB2	2.02	0.41
1:C:185:ASN:O	1:C:187:GLN:N	2.53	0.41
1:A:1:MET:N	5:A:432:HOH:O	2.35	0.41
1:A:129:ILE:HD12	1:A:152:LEU:HD23	2.03	0.41
1:B:97:PRO:HG2	1:B:109:MET:SD	2.61	0.41
1:B:370:ILE:HG23	5:B:664:HOH:O	2.20	0.41
1:C:228:ILE:HD12	1:C:256:ILE:O	2.21	0.41
1:C:381:MET:HE3	1:C:381:MET:HB3	1.91	0.41
1:D:99:THR:CG2	1:D:109:MET:HB2	2.51	0.41
1:A:56:GLU:HB2	1:B:49:LYS:HE3	2.03	0.40
1:B:155:ASN:HB2	5:B:709:HOH:O	2.20	0.40
1:B:240:LYS:NZ	5:B:672:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:LEU:HD22	1:D:414:PHE:CD2	2.56	0.40
1:A:168:PRO:HD2	5:A:634:HOH:O	2.21	0.40
1:D:181:GLU:CD	1:D:181:GLU:H	2.24	0.40
1:B:58:GLY:HA2	5:B:432:HOH:O	2.20	0.40
1:C:8:THR:HG23	1:C:10:ALA:H	1.87	0.40
1:D:278:LYS:HG3	5:D:720:HOH:O	2.20	0.40
1:A:167:VAL:HA	1:A:168:PRO:HD3	1.91	0.40
1:B:123:LYS:NZ	5:B:616:HOH:O	2.44	0.40
1:B:283:ARG:HD3	5:B:580:HOH:O	2.21	0.40
1:B:328:ASN:ND2	5:B:661:HOH:O	2.48	0.40
1:C:326:TYR:CE1	1:C:354:MET:HE2	2.56	0.40
1:A:39:GLY:HA3	3:A:427:KYN:HA	2.04	0.40
1:C:49:LYS:HE3	1:D:56:GLU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	423/425 (100%)	402 (95%)	12 (3%)	9 (2%)	7 1
1	B	423/425 (100%)	409 (97%)	13 (3%)	1 (0%)	47 38
1	C	423/425 (100%)	405 (96%)	15 (4%)	3 (1%)	22 11
1	D	423/425 (100%)	408 (96%)	12 (3%)	3 (1%)	22 11
All	All	1692/1700 (100%)	1624 (96%)	52 (3%)	16 (1%)	17 8

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	PRO
1	A	19	ILE

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Mol	Chain	Res	Type
1	A	182	ASP
1	A	184	LYS
1	B	17	SER
1	C	18	PRO
1	C	19	ILE
1	D	18	PRO
1	D	19	ILE
1	A	17	SER
1	A	189	ASN
1	C	186	PRO
1	D	266	SER
1	A	187	GLN
1	A	186	PRO
1	A	18	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	370/370 (100%)	330 (89%)	40 (11%)	6 1
1	B	370/370 (100%)	337 (91%)	33 (9%)	9 2
1	C	370/370 (100%)	337 (91%)	33 (9%)	9 2
1	D	370/370 (100%)	339 (92%)	31 (8%)	11 3
All	All	1480/1480 (100%)	1343 (91%)	137 (9%)	9 2

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	THR
1	A	17	SER
1	A	19	ILE
1	A	22	MET
1	A	28	ARG
1	A	60	THR

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Mol	Chain	Res	Type
1	A	87	LEU
1	A	99	THR
1	A	106	GLN
1	A	137	LEU
1	A	152	LEU
1	A	166	ILE
1	A	177	ARG
1	A	179	LYS
1	A	181	GLU
1	A	184	LYS
1	A	187	GLN
1	A	192	LYS
1	A	218	GLU
1	A	221	ARG
1	A	226	LEU
1	A	228	ILE
1	A	243	VAL
1	A	288	ILE
1	A	297	THR
1	A	301	LEU
1	A	307	LEU
1	A	309	GLU
1	A	313	GLU
1	A	316	MET
1	A	320	ASP
1	A	322	VAL
1	A	334	LEU
1	A	341	LEU
1	A	342	THR
1	A	344	LEU
1	A	364	ASN
1	A	415	GLN
1	A	417	LEU
1	B	20	ARG
1	B	42	ASN
1	B	59	LYS
1	B	60	THR
1	B	65	GLU
1	B	83	LEU
1	B	84	LEU
1	B	87	LEU
1	B	99	THR

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Mol	Chain	Res	Type
1	B	145	THR
1	B	166	ILE
1	B	187	GLN
1	B	203	PRO
1	B	218	GLU
1	B	219	LEU
1	B	226	LEU
1	B	228	ILE
1	B	236	LEU
1	B	243	VAL
1	B	278	LYS
1	B	280	LEU
1	B	283	ARG
1	B	284	VAL
1	B	297	THR
1	B	301	LEU
1	B	307	LEU
1	B	309	GLU
1	B	322	VAL
1	B	334	LEU
1	B	341	LEU
1	B	360	VAL
1	B	385	ASN
1	B	417	LEU
1	C	1	MET
1	C	8	THR
1	C	20	ARG
1	C	24	ASP
1	C	28	ARG
1	C	31	LYS
1	C	52	VAL
1	C	60	THR
1	C	87	LEU
1	C	93	LYS
1	C	94	LEU
1	C	118	GLN
1	C	137	LEU
1	C	152	LEU
1	C	166	ILE
1	C	174	ILE
1	C	178	TRP
1	C	179	LYS

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Mol	Chain	Res	Type
1	C	219	LEU
1	C	221	ARG
1	C	226	LEU
1	C	236	LEU
1	C	239	ASN
1	C	243	VAL
1	C	278	LYS
1	C	297	THR
1	C	307	LEU
1	C	322	VAL
1	C	334	LEU
1	C	344	LEU
1	C	376	LYS
1	C	415	GLN
1	C	417	LEU
1	D	8	THR
1	D	28	ARG
1	D	60	THR
1	D	83	LEU
1	D	87	LEU
1	D	99	THR
1	D	137	LEU
1	D	152	LEU
1	D	174	ILE
1	D	177	ARG
1	D	185	ASN
1	D	203	PRO
1	D	219	LEU
1	D	221	ARG
1	D	226	LEU
1	D	228	ILE
1	D	236	LEU
1	D	243	VAL
1	D	278	LYS
1	D	280	LEU
1	D	283	ARG
1	D	284	VAL
1	D	297	THR
1	D	307	LEU
1	D	313	GLU
1	D	319	VAL
1	D	327	SER

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Mol	Chain	Res	Type
1	D	334	LEU
1	D	341	LEU
1	D	376	LYS
1	D	417	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	95	HIS
1	A	118	GLN
1	A	185	ASN
1	A	201	ASN
1	A	206	ASN
1	A	237	GLN
1	A	294	HIS
1	A	305	GLN
1	A	318	HIS
1	B	2	ASN
1	B	42	ASN
1	B	108	GLN
1	B	187	GLN
1	B	201	ASN
1	B	206	ASN
1	B	294	HIS
1	B	299	ASN
1	B	305	GLN
1	B	308	HIS
1	B	348	HIS
1	B	364	ASN
1	C	2	ASN
1	C	57	ASN
1	C	91	GLN
1	C	95	HIS
1	C	96	ASN
1	C	108	GLN
1	C	118	GLN
1	C	187	GLN
1	C	201	ASN
1	C	237	GLN
1	C	294	HIS
1	C	299	ASN

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Mol	Chain	Res	Type
1	C	305	GLN
1	C	318	HIS
1	C	328	ASN
1	C	419	GLN
1	D	57	ASN
1	D	106	GLN
1	D	108	GLN
1	D	185	ASN
1	D	201	ASN
1	D	237	GLN
1	D	294	HIS
1	D	299	ASN
1	D	305	GLN
1	D	308	HIS
1	D	364	ASN
1	D	419	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
4	GOL	D	429	-	5,5,5	0.66	0	5,5,5	0.70	0
3	KYN	A	427	-	13,15,15	1.85	2 (15%)	17,20,20	1.50	4 (23%)
4	GOL	D	427	-	5,5,5	0.55	0	5,5,5	0.98	0
2	PMP	D	426	-	16,16,16	1.28	2 (12%)	21,23,23	1.39	4 (19%)
3	KYN	A	428	-	13,15,15	1.70	1 (7%)	17,20,20	1.02	1 (5%)
4	GOL	C	429	-	5,5,5	0.79	0	5,5,5	0.76	0
4	GOL	A	429	-	5,5,5	1.16	1 (20%)	5,5,5	1.10	1 (20%)
3	KYN	C	428	-	13,15,15	1.48	2 (15%)	17,20,20	1.41	4 (23%)
4	GOL	D	430	-	5,5,5	0.47	0	5,5,5	0.59	0
2	PMP	B	426	-	16,16,16	1.29	1 (6%)	21,23,23	1.40	3 (14%)
2	PMP	C	426	-	16,16,16	1.25	2 (12%)	21,23,23	1.39	3 (14%)
2	PMP	A	426	-	16,16,16	1.28	2 (12%)	21,23,23	1.56	4 (19%)
3	KYN	C	427	-	13,15,15	1.47	2 (15%)	17,20,20	1.25	2 (11%)
4	GOL	D	428	-	5,5,5	0.47	0	5,5,5	0.83	0

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
4	GOL	D	429	-	-	4/4/4/4	-
3	KYN	A	427	-	-	7/12/12/12	0/1/1/1
4	GOL	D	427	-	-	2/4/4/4	-
2	PMP	D	426	-	-	5/8/8/8	0/1/1/1
3	KYN	A	428	-	-	7/12/12/12	0/1/1/1
4	GOL	C	429	-	-	0/4/4/4	-
4	GOL	A	429	-	-	0/4/4/4	-
3	KYN	C	428	-	-	6/12/12/12	0/1/1/1
4	GOL	D	430	-	-	3/4/4/4	-
2	PMP	B	426	-	-	5/8/8/8	0/1/1/1
2	PMP	C	426	-	-	3/8/8/8	0/1/1/1
2	PMP	A	426	-	-	7/8/8/8	0/1/1/1
3	KYN	C	427	-	-	4/12/12/12	0/1/1/1
4	GOL	D	428	-	-	4/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	428	KYN	OXT-C	-5.51	1.12	1.30
3	A	427	KYN	OXT-C	4.90	1.46	1.30
3	C	428	KYN	OXT-C	-4.41	1.16	1.30
3	C	427	KYN	OXT-C	-4.26	1.16	1.30
3	A	427	KYN	CD2-CG	-3.95	1.36	1.41
2	B	426	PMP	C2-N1	3.47	1.40	1.33
2	C	426	PMP	C2-N1	3.15	1.39	1.33
2	A	426	PMP	C2-N1	3.14	1.39	1.33
2	D	426	PMP	C2-N1	3.08	1.39	1.33
2	D	426	PMP	C6-N1	2.64	1.40	1.34
3	C	427	KYN	CD2-CG	-2.57	1.38	1.41
2	A	426	PMP	C6-N1	2.57	1.39	1.34
2	C	426	PMP	C6-N1	2.53	1.39	1.34
4	A	429	GOL	O2-C2	-2.39	1.36	1.43
3	C	428	KYN	CD2-CG	-2.38	1.38	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	426	PMP	O2P-P-O4P	3.37	115.71	106.73
2	B	426	PMP	C3-C4-C5	3.16	121.75	118.72
3	C	427	KYN	CA-CB-C1	-3.16	109.68	113.70
3	A	427	KYN	CD2-CG-N1	-3.11	118.56	122.67
3	C	428	KYN	CD1-CG-CD2	3.00	121.01	118.10
2	D	426	PMP	O2P-P-O4P	2.98	114.66	106.73
2	A	426	PMP	C2A-C2-C3	-2.84	117.38	120.89
2	C	426	PMP	C3-C4-C5	2.70	121.31	118.72
3	C	427	KYN	CD1-CG-CD2	2.63	120.64	118.10
2	C	426	PMP	C4A-C4-C3	-2.56	116.27	120.34
2	A	426	PMP	C2A-C2-N1	2.55	122.66	117.67
3	A	427	KYN	CD1-CG-CD2	2.46	120.48	118.10
2	A	426	PMP	O3P-P-O2P	2.44	116.98	107.64
2	B	426	PMP	O2P-P-O4P	2.41	113.15	106.73
2	B	426	PMP	C5-C6-N1	-2.41	119.80	123.82
3	C	428	KYN	OXT-C-CA	2.38	121.50	113.38
3	C	428	KYN	CA-CB-C1	-2.36	110.69	113.70
2	D	426	PMP	C4A-C4-C3	-2.31	116.67	120.34
3	C	428	KYN	CD2-CG-N1	-2.15	119.83	122.67
2	D	426	PMP	O3P-P-O2P	2.14	115.82	107.64
3	A	428	KYN	CA-CB-C1	-2.13	110.98	113.70
4	A	429	GOL	O2-C2-C3	-2.12	99.77	109.12
3	A	427	KYN	CE2-CD2-CG	2.12	121.17	118.93
3	A	427	KYN	O2-C1-CB	2.07	123.16	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	426	PMP	O2P-P-O1P	2.06	118.75	110.68
2	D	426	PMP	C3-C4-C5	2.01	120.64	118.72

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	426	PMP	C5A-O4P-P-O1P
2	A	426	PMP	C5A-O4P-P-O2P
2	A	426	PMP	C5A-O4P-P-O3P
2	B	426	PMP	C3-C4-C4A-N4A
2	B	426	PMP	C5A-O4P-P-O2P
2	B	426	PMP	C5A-O4P-P-O3P
2	C	426	PMP	C5A-O4P-P-O1P
2	C	426	PMP	C5A-O4P-P-O2P
2	C	426	PMP	C5A-O4P-P-O3P
2	D	426	PMP	C3-C4-C4A-N4A
2	D	426	PMP	C5-C4-C4A-N4A
2	D	426	PMP	C5A-O4P-P-O1P
3	A	428	KYN	C-CA-CB-C1
4	D	427	GOL	O1-C1-C2-C3
4	D	428	GOL	O1-C1-C2-C3
4	D	428	GOL	C1-C2-C3-O3
2	A	426	PMP	C3-C4-C4A-N4A
4	D	430	GOL	O1-C1-C2-O2
3	A	427	KYN	CB-C1-CD2-CE2
4	D	429	GOL	O1-C1-C2-C3
4	D	429	GOL	C1-C2-C3-O3
4	D	430	GOL	O1-C1-C2-C3
2	A	426	PMP	C5-C4-C4A-N4A
2	B	426	PMP	C5-C4-C4A-N4A
4	D	427	GOL	O1-C1-C2-O2
4	D	428	GOL	O1-C1-C2-O2
4	D	429	GOL	O2-C2-C3-O3
3	A	427	KYN	O2-C1-CD2-CE2
3	A	428	KYN	N-CA-CB-C1
3	A	427	KYN	O2-C1-CB-CA
3	A	428	KYN	O2-C1-CB-CA
3	C	427	KYN	O2-C1-CB-CA
3	C	428	KYN	O2-C1-CB-CA
3	A	427	KYN	CD2-C1-CB-CA
3	A	428	KYN	CD2-C1-CB-CA

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Mol	Chain	Res	Type	Atoms
3	C	427	KYN	CD2-C1-CB-CA
3	C	428	KYN	CD2-C1-CB-CA
4	D	428	GOL	O2-C2-C3-O3
3	A	428	KYN	OXT-C-CA-N
2	B	426	PMP	C5A-O4P-P-O1P
3	A	427	KYN	O2-C1-CD2-CG
3	C	428	KYN	O2-C1-CD2-CG
3	C	428	KYN	O2-C1-CD2-CE2
3	A	427	KYN	CB-C1-CD2-CG
3	A	428	KYN	O-C-CA-N
3	C	428	KYN	CB-C1-CD2-CE2
2	A	426	PMP	C4-C5-C5A-O4P
2	D	426	PMP	C4-C5-C5A-O4P
4	D	430	GOL	O2-C2-C3-O3
3	C	427	KYN	O2-C1-CD2-CE2
3	A	427	KYN	N-CA-CB-C1
4	D	429	GOL	O1-C1-C2-O2
3	C	427	KYN	O2-C1-CD2-CG
3	A	428	KYN	O2-C1-CD2-CE2
3	C	428	KYN	CB-C1-CD2-CG
2	A	426	PMP	C6-C5-C5A-O4P
2	D	426	PMP	C6-C5-C5A-O4P

There are no ring outliers.

13 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	429	GOL	4	0
3	A	427	KYN	4	0
4	D	427	GOL	4	0
2	D	426	PMP	4	0
4	C	429	GOL	6	0
4	A	429	GOL	6	0
3	C	428	KYN	2	0
4	D	430	GOL	1	0
2	B	426	PMP	2	0
2	C	426	PMP	2	0
2	A	426	PMP	3	0
3	C	427	KYN	3	0
4	D	428	GOL	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	425/425 (100%)	0.18	26 (6%)	21	29	18, 29, 52, 78	0
1	B	425/425 (100%)	0.16	22 (5%)	27	37	18, 29, 46, 78	0
1	C	425/425 (100%)	0.05	17 (4%)	38	48	14, 23, 43, 85	0
1	D	425/425 (100%)	-0.07	17 (4%)	38	48	14, 22, 39, 79	0
All	All	1700/1700 (100%)	0.08	82 (4%)	30	40	14, 26, 46, 85	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	17	SER	9.6
1	C	20	ARG	8.4
1	C	21	THR	8.0
1	C	19	ILE	7.5
1	A	17	SER	6.4
1	C	186	PRO	6.4
1	D	19	ILE	6.3
1	D	21	THR	5.9
1	D	23	THR	5.8
1	C	24	ASP	5.4
1	C	25	ILE	5.3
1	D	17	SER	5.1
1	B	17	SER	5.0
1	A	20	ARG	5.0
1	B	18	PRO	5.0
1	A	19	ILE	4.8
1	B	20	ARG	4.8
1	D	20	ARG	4.8
1	B	21	THR	4.8
1	D	18	PRO	4.6
1	C	23	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	342	THR	4.4
1	D	22	MET	4.3
1	C	22	MET	4.3
1	B	24	ASP	4.1
1	A	18	PRO	4.1
1	D	28	ARG	4.0
1	A	24	ASP	3.7
1	A	23	THR	3.7
1	D	187	GLN	3.7
1	C	18	PRO	3.6
1	A	184	LYS	3.5
1	B	19	ILE	3.5
1	A	179	LYS	3.5
1	B	26	LEU	3.3
1	D	425	LEU	3.2
1	A	21	THR	3.2
1	D	31	LYS	3.2
1	B	28	ARG	3.1
1	B	25	ILE	3.1
1	A	27	SER	3.1
1	D	24	ASP	3.0
1	B	57	ASN	2.9
1	B	371	GLU	2.9
1	B	23	THR	2.9
1	B	425	LEU	2.9
1	C	28	ARG	2.8
1	C	26	LEU	2.7
1	B	27	SER	2.7
1	C	31	LYS	2.7
1	A	31	LYS	2.6
1	B	187	GLN	2.6
1	B	31	LYS	2.5
1	B	226	LEU	2.5
1	D	29	GLY	2.5
1	A	187	GLN	2.4
1	B	228	ILE	2.4
1	D	241	PHE	2.4
1	D	27	SER	2.4
1	A	16	PRO	2.3
1	A	194	LEU	2.2
1	A	29	GLY	2.2
1	C	239	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	27	SER	2.2
1	B	188	LYS	2.2
1	B	22	MET	2.2
1	C	16	PRO	2.2
1	D	26	LEU	2.2
1	A	183	ALA	2.2
1	A	221	ARG	2.2
1	A	197	VAL	2.2
1	A	186	PRO	2.1
1	A	265	ILE	2.1
1	A	57	ASN	2.1
1	A	22	MET	2.1
1	D	239	ASN	2.1
1	A	28	ARG	2.0
1	A	181	GLU	2.0
1	C	241	PHE	2.0
1	A	182	ASP	2.0
1	B	194	LEU	2.0
1	B	398	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	KYN	C	427	15/15	0.65	0.28	61,63,69,69	0
3	KYN	C	428	15/15	0.70	0.31	62,65,72,72	0
3	KYN	A	428	15/15	0.75	0.26	62,65,69,69	0
4	GOL	C	429	6/6	0.79	0.24	33,34,36,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	KYN	A	427	15/15	0.81	0.27	66,69,74,75	0
4	GOL	D	429	6/6	0.83	0.27	35,39,40,41	0
4	GOL	D	430	6/6	0.83	0.41	39,43,44,45	0
4	GOL	D	427	6/6	0.88	0.26	21,32,36,42	0
4	GOL	A	429	6/6	0.89	0.28	26,33,34,34	0
4	GOL	D	428	6/6	0.89	0.21	25,37,42,45	0
2	PMP	B	426	16/16	0.94	0.13	29,36,40,44	0
2	PMP	A	426	16/16	0.95	0.11	28,33,36,39	0
2	PMP	C	426	16/16	0.96	0.11	20,28,34,38	0
2	PMP	D	426	16/16	0.96	0.10	18,32,36,38	0

6.5 Other polymers (i)

There are no such residues in this entry.