



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 10:51 PM EDT

PDB ID : 6ED7  
Title : Crystal structure of 7,8-diaminopelargonic acid synthase bound to inhibitor MAC13772  
Authors : Brown, C.M.; Zlitni, S.; Chan, J.; Brown, E.D.; Junop, M.S.  
Deposited on : 2018-08-08  
Resolution : 2.43 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.37.1  
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) : 2.37.1

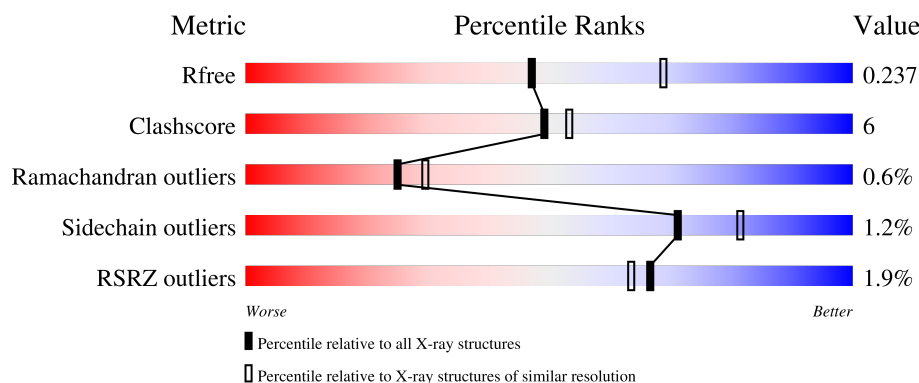
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*






The reported resolution of this entry is 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	429	 86% 13% .
1	B	429	 86% 14%
1	C	429	 81% 18%
1	D	429	 88% 12%
1	E	429	 86% 13% .

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Mol	Chain	Length	Quality of chain
1	F	429	<div><div>%</div><div><div></div><div>86%</div><div>13%</div><div></div></div><div></div></div>
1	G	429	<div><div>5%</div><div><div></div><div>84%</div><div>14%</div><div></div></div><div></div></div>
1	H	429	<div><div>2%</div><div><div></div><div>85%</div><div>14%</div><div></div></div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27268 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 7,8-diamino-pelargonic acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3272	2078	567	597	30			
1	B	429	Total	C	N	O	S	0	0	0
			3290	2088	574	597	31			
1	C	429	Total	C	N	O	S	0	0	0
			3236	2059	557	590	30			
1	D	429	Total	C	N	O	S	0	0	0
			3283	2084	572	596	31			
1	E	429	Total	C	N	O	S	0	0	0
			3254	2069	562	593	30			
1	F	429	Total	C	N	O	S	0	0	0
			3261	2071	567	593	30			
1	G	429	Total	C	N	O	S	0	0	0
			3218	2046	559	582	31			
1	H	429	Total	C	N	O	S	0	0	0
			3261	2072	565	593	31			

There are 8 discrepancies between the modelled and reference sequences:

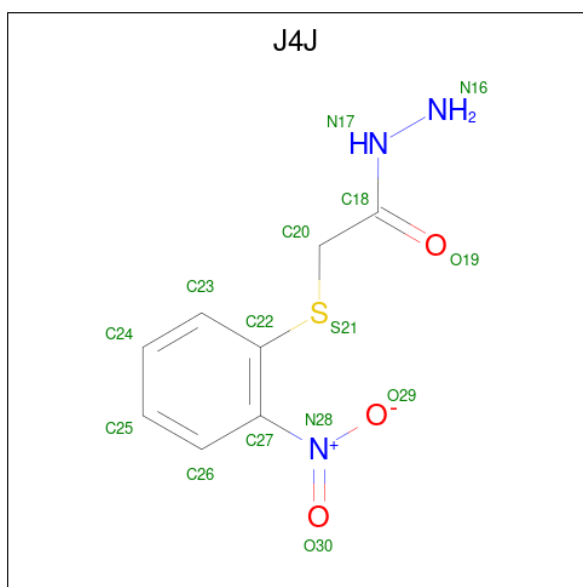
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP A0A0A0GYM0
B	1	ALA	-	expression tag	UNP A0A0A0GYM0
C	1	ALA	-	expression tag	UNP A0A0A0GYM0
D	1	ALA	-	expression tag	UNP A0A0A0GYM0
E	1	ALA	-	expression tag	UNP A0A0A0GYM0
F	1	ALA	-	expression tag	UNP A0A0A0GYM0
G	1	ALA	-	expression tag	UNP A0A0A0GYM0
H	1	ALA	-	expression tag	UNP A0A0A0GYM0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 2-[(2-nitrophenyl)sulfanyl]acetohydrazide (three-letter code: J4J) (formula:  $C_8H_9N_3O_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	3	3	1		
3	A	1	Total	C	N	O	S	0	0
			15	8	3	3	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	3	3	1		
3	B	1	Total	C	N	O	S	0	0
			14	8	3	2	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	3	3	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	3	3	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	3	3	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	3	3	1		
3	E	1	Total	C	N	O	S	0	0
			15	8	3	3	1		
3	E	1	Total	C	N	O	S	0	0
			15	8	3	3	1		
3	F	1	Total	C	N	O	S	0	0
			15	8	3	3	1		
3	F	1	Total	C	N	O	S	0	0
			15	8	3	3	1		
3	G	1	Total	C	N	O	S	0	0
			15	8	3	3	1		
3	G	1	Total	C	N	O	S	0	0
			15	8	3	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	N	O	S	0	0
			15	8	3	3	1		
3	H	1	Total	C	N	O	S	0	0
			15	8	3	3	1		

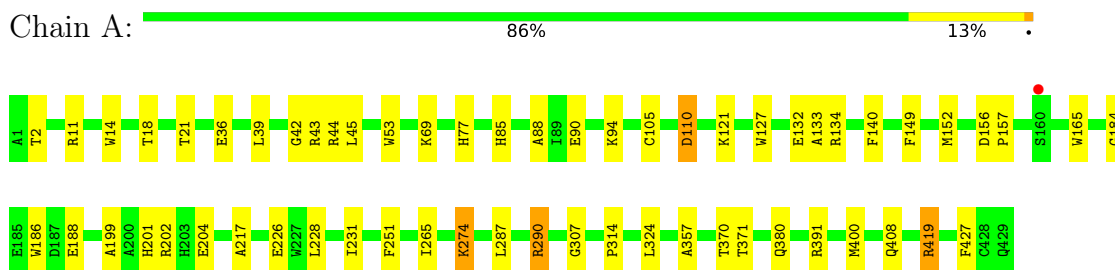
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	145	Total	O	0	0
			145	145		
4	C	100	Total	O	0	0
			100	100		
4	D	127	Total	O	0	0
			127	127		
4	E	102	Total	O	0	0
			102	102		
4	F	97	Total	O	0	0
			97	97		
4	G	64	Total	O	0	0
			64	64		
4	H	82	Total	O	0	0
			82	82		

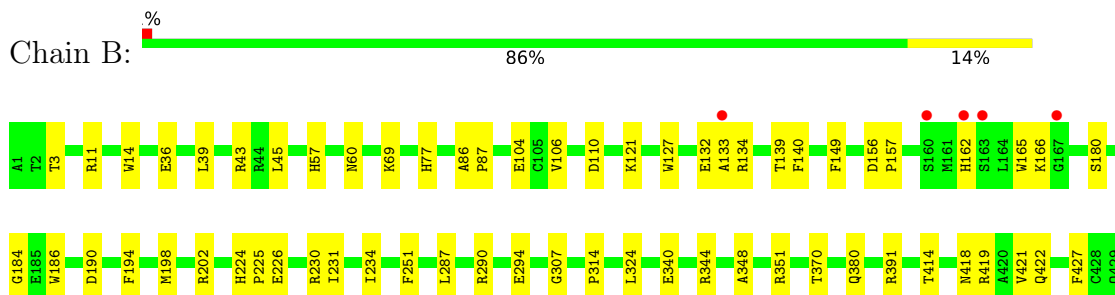
### 3 Residue-property plots

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.

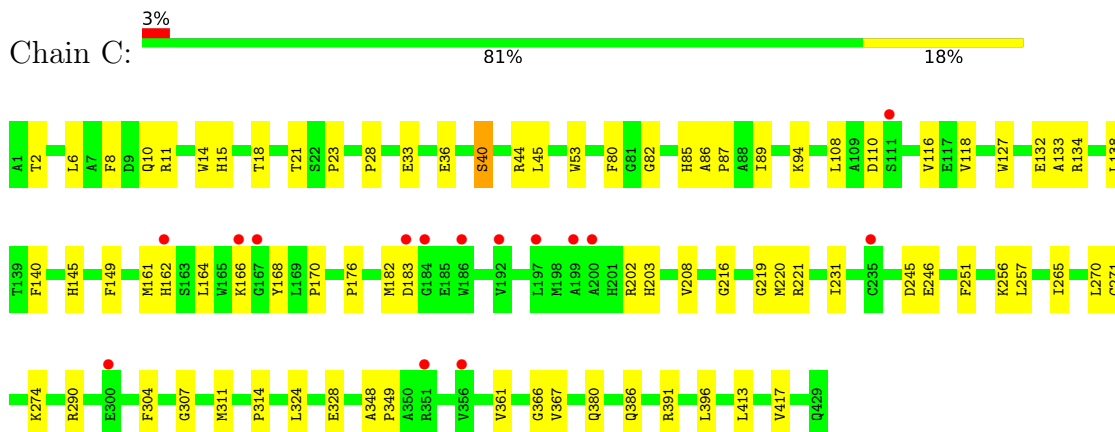
- Molecule 1: 7,8-diamino-pelargonic acid aminotransferase



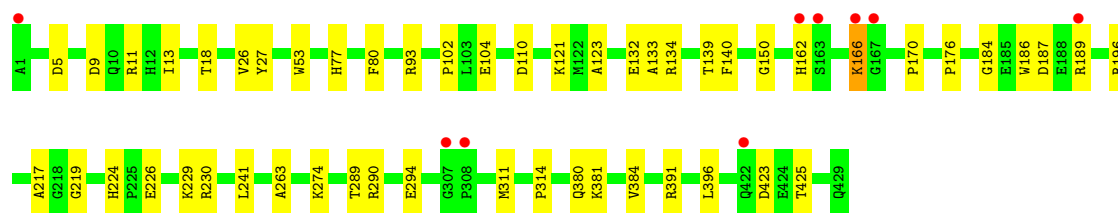
- Molecule 1: 7,8-diamino-pelargonic acid aminotransferase



- Molecule 1: 7,8-diamino-pelargonic acid aminotransferase

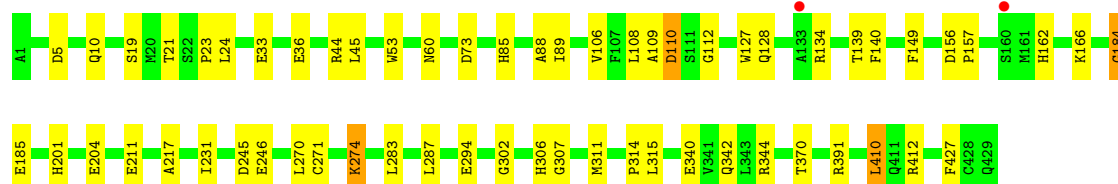






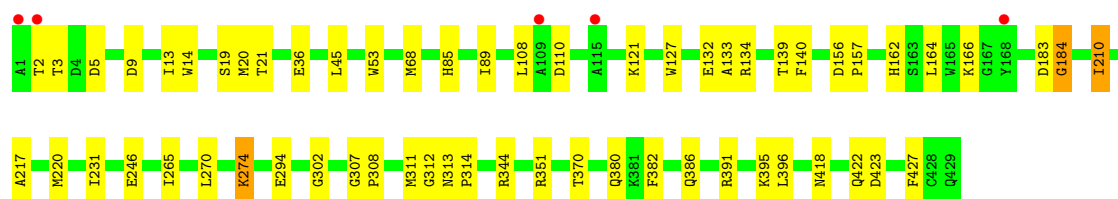
- Molecule 1: 7,8-diamino-pelargonic acid aminotransferase

Chain E: 86% 13%



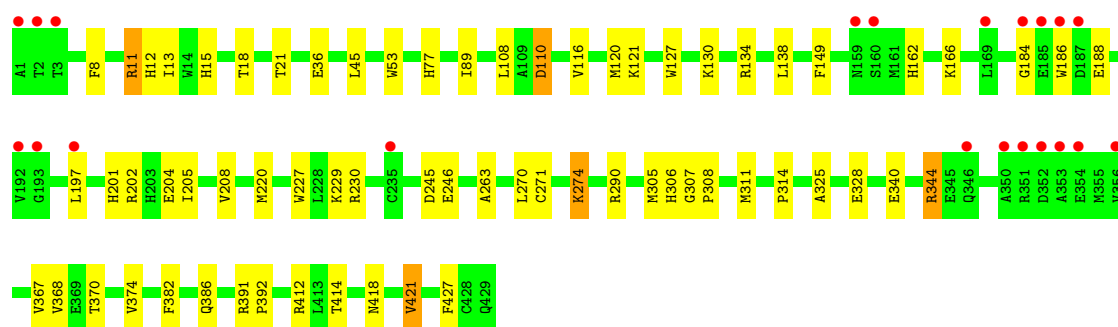
- Molecule 1: 7,8-diamino-pelargonic acid aminotransferase

Chain F: 86% 13%



- Molecule 1: 7,8-diamino-pelargonic acid aminotransferase

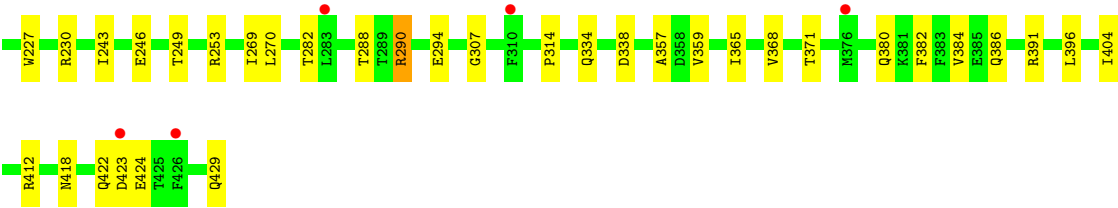
Chain G: 84% 14% 2%



- Molecule 1: 7,8-diamino-pelargonic acid aminotransferase

Chain H: 85% 14% 2%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.43Å 111.57Å 136.12Å 90.00° 92.08° 90.00°	Depositor
Resolution (Å)	42.79 – 2.43 42.79 – 2.43	Depositor EDS
% Data completeness (in resolution range)	75.6 (42.79-2.43) 75.6 (42.79-2.43)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.177 , 0.237 0.176 , 0.237	Depositor DCC
$R_{free}$ test set	5304 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	27268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, J4J

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	0.50	0/3351	0.61	0/4558
1	B	0.52	0/3369	0.62	0/4579
1	C	0.45	0/3315	0.59	0/4516
1	D	0.47	0/3362	0.61	0/4570
1	E	0.45	0/3333	0.61	1/4536 (0.0%)
1	F	0.46	0/3340	0.60	1/4543 (0.0%)
1	G	0.38	0/3296	0.58	2/4487 (0.0%)
1	H	0.41	0/3340	0.59	0/4542
All	All	0.45	0/26706	0.60	4/36331 (0.0%)

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	1
1	B	0	1
1	G	0	1
1	H	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	344	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	E	412	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	F	351	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	G	344	ARG	NE-CZ-NH1	-5.70	117.45	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	GLY	Peptide
1	B	184	GLY	Peptide
1	G	184	GLY	Peptide
1	H	184	GLY	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3272	0	3190	39	0
1	B	3290	0	3222	34	0
1	C	3236	0	3125	54	0
1	D	3283	0	3213	34	0
1	E	3254	0	3160	41	0
1	F	3261	0	3163	43	0
1	G	3218	0	3113	48	0
1	H	3261	0	3174	42	0
2	A	15	0	7	1	0
2	B	15	0	6	0	0
2	C	15	0	6	0	0
2	D	15	0	6	1	0
2	E	15	0	6	2	0
2	F	15	0	7	0	0
2	G	15	0	6	0	0
2	H	15	0	7	0	0
3	A	30	0	0	3	0
3	B	29	0	0	0	0
3	C	30	0	0	2	0
3	D	30	0	0	2	0
3	E	30	0	0	3	0
3	F	30	0	0	2	0
3	G	30	0	0	2	0
3	H	30	0	0	3	0
4	A	117	0	0	7	0
4	B	145	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	100	0	0	9	0
4	D	127	0	0	4	0
4	E	102	0	0	4	0
4	F	97	0	0	4	0
4	G	64	0	0	2	0
4	H	82	0	0	3	0
All	All	27268	0	25411	304	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 6.

All (304) 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:G:340:GLU:HG2	1:G:344:ARG:HH12	1.26	0.97
1:A:11:ARG:O	1:B:290:ARG:NH1	2.03	0.91
1:C:161:MET:O	4:C:701:HOH:O	2.02	0.77
1:C:127:TRP:CD2	1:C:134:ARG:HD2	2.22	0.74
1:H:391:ARG:HH21	3:H:603:J4J:C25	2.00	0.73
1:G:340:GLU:HG2	1:G:344:ARG:NH1	2.04	0.72
1:C:391:ARG:HH21	3:C:603:J4J:C25	2.04	0.70
1:E:391:ARG:HH21	3:E:603:J4J:C25	2.05	0.69
1:A:391:ARG:HE	3:A:603:J4J:C25	2.05	0.69
1:G:134:ARG:NH1	1:G:202:ARG:O	2.25	0.69
1:C:256:LYS:O	4:C:702:HOH:O	2.12	0.68
1:G:391:ARG:HH21	3:G:602:J4J:C25	2.06	0.67
2:A:601:PLP:O1P	4:A:701:HOH:O	2.13	0.67
1:E:127:TRP:CD2	1:E:134:ARG:HD2	2.30	0.66
1:D:162:HIS:O	1:D:166:LYS:N	2.27	0.65
1:C:140:PHE:HZ	1:C:231:ILE:HD11	1.62	0.65
1:F:127:TRP:CD2	1:F:134:ARG:HD2	2.32	0.65
1:G:53:TRP:HB2	1:G:274:LYS:HD3	1.78	0.64
1:E:162:HIS:O	1:E:166:LYS:N	2.28	0.64
1:F:162:HIS:O	1:F:166:LYS:N	2.30	0.64
1:B:162:HIS:O	1:B:166:LYS:N	2.31	0.63
1:D:187:ASP:OD2	1:D:189:ARG:NH2	2.29	0.63
1:D:77:HIS:HA	1:D:314:PRO:HD2	1.81	0.62
1:F:391:ARG:HE	3:F:603:J4J:C25	2.13	0.62
1:A:127:TRP:CD2	1:A:134:ARG:HD2	2.35	0.61
1:D:391:ARG:HH21	3:D:603:J4J:C25	2.12	0.61
1:E:85:HIS:CE1	1:E:314:PRO:HG3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PHE:HZ	1:A:231:ILE:HD11	1.64	0.61
1:G:414:THR:O	1:G:418:ASN:ND2	2.34	0.61
1:G:246:GLU:HG3	1:G:270:LEU:HD11	1.83	0.60
1:D:27:TYR:CE2	1:D:384:VAL:HG21	2.36	0.60
1:G:340:GLU:CG	1:G:344:ARG:HH12	2.08	0.60
1:G:344:ARG:HG3	1:G:344:ARG:HH11	1.66	0.60
1:C:140:PHE:CZ	1:C:231:ILE:HD11	2.37	0.59
1:E:294:GLU:HG2	1:F:21:THR:HG22	1.82	0.59
1:A:290:ARG:NH2	1:B:11:ARG:O	2.20	0.59
1:A:201:HIS:ND1	1:A:204:GLU:OE2	2.30	0.59
1:D:196:ARG:NH2	4:D:707:HOH:O	2.36	0.59
1:E:306:HIS:NE2	4:E:704:HOH:O	2.27	0.59
1:A:42:GLY:O	4:A:702:HOH:O	2.16	0.59
1:C:246:GLU:HG3	1:C:270:LEU:HD11	1.84	0.58
1:C:21:THR:HG22	1:D:294:GLU:HG2	1.85	0.58
1:E:184:GLY:HA2	1:E:185:GLU:CB	2.32	0.58
1:A:357:ALA:HB2	1:A:371:THR:HG22	1.86	0.58
1:F:53:TRP:HB2	1:F:274:LYS:HD3	1.84	0.58
1:H:380:GLN:OE1	1:H:391:ARG:HD2	2.04	0.58
1:C:89:ILE:HD13	1:D:5:ASP:HB3	1.86	0.58
1:H:104:GLU:OE1	1:H:290:ARG:NH2	2.36	0.58
1:B:414:THR:O	1:B:418:ASN:ND2	2.37	0.57
1:H:189:ARG:O	1:H:192:VAL:HG13	2.05	0.57
1:E:112:GLY:HA3	2:E:601:PLP:H5A2	1.86	0.57
1:H:382:PHE:O	1:H:386:GLN:HG2	2.04	0.57
1:G:21:THR:HG22	1:H:294:GLU:HG2	1.87	0.56
1:H:246:GLU:HG3	1:H:270:LEU:HD11	1.88	0.56
1:C:380:GLN:OE1	1:C:391:ARG:HD2	2.07	0.55
1:H:25:PRO:HG2	4:H:756:HOH:O	2.07	0.55
1:H:162:HIS:O	1:H:166:LYS:N	2.39	0.55
1:E:73:ASP:OD2	4:E:701:HOH:O	2.18	0.55
1:C:361:VAL:HG22	1:C:366:GLY:HA2	1.89	0.55
1:C:386:GLN:NE2	4:C:707:HOH:O	2.39	0.55
1:G:344:ARG:NH1	1:G:344:ARG:HG3	2.22	0.55
1:G:229:LYS:HG3	1:G:263:ALA:HB1	1.89	0.55
1:H:412:ARG:NH2	4:H:709:HOH:O	2.40	0.55
1:A:380:GLN:OE1	1:A:391:ARG:HD2	2.06	0.54
1:A:110:ASP:OD2	1:A:110:ASP:N	2.41	0.53
1:F:246:GLU:HG3	1:F:270:LEU:HD11	1.88	0.53
1:A:44:ARG:NH1	4:A:708:HOH:O	2.40	0.53
1:C:176:PRO:O	4:C:703:HOH:O	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:THR:OG1	1:D:140:PHE:N	2.41	0.53
1:C:138:LEU:HB3	1:C:208:VAL:HG22	1.90	0.53
1:C:11:ARG:O	1:D:290:ARG:NH1	2.28	0.53
1:C:8:PHE:CZ	1:D:93:ARG:HA	2.44	0.53
1:E:53:TRP:HB2	1:E:274:LYS:HD3	1.91	0.53
1:B:162:HIS:HA	1:B:165:TRP:HD1	1.73	0.53
1:C:274:LYS:HZ1	3:C:602:J4J:C18	2.22	0.53
1:E:128:GLN:NE2	1:F:164:LEU:O	2.41	0.52
1:C:168:TYR:O	4:C:704:HOH:O	2.18	0.52
1:C:162:HIS:O	1:C:166:LYS:N	2.37	0.52
1:E:315:LEU:HD22	1:F:68:MET:HE1	1.91	0.52
1:H:139:THR:OG1	1:H:140:PHE:N	2.43	0.52
1:F:220:MET:HG2	1:F:396:LEU:HD13	1.92	0.52
1:A:85:HIS:CD2	1:A:88:ALA:H	2.27	0.52
1:E:89:ILE:HD13	1:F:5:ASP:HB3	1.92	0.52
1:A:85:HIS:HD2	1:A:88:ALA:H	1.56	0.52
1:A:391:ARG:HH21	3:A:603:J4J:C25	2.22	0.52
1:E:140:PHE:HZ	1:E:231:ILE:HD11	1.74	0.52
1:C:85:HIS:CE1	1:C:314:PRO:HG3	2.46	0.51
1:A:228:LEU:HB3	1:A:265:ILE:HG12	1.93	0.51
1:B:39:LEU:HD12	1:B:43:ARG:HD2	1.92	0.51
1:B:57:HIS:O	4:B:701:HOH:O	2.19	0.51
1:B:127:TRP:CD2	1:B:134:ARG:HD2	2.46	0.51
1:E:10:GLN:NE2	4:E:703:HOH:O	2.24	0.51
1:C:290:ARG:NH2	1:D:11:ARG:O	2.36	0.51
1:A:217:ALA:HB1	3:A:602:J4J:C25	2.41	0.50
1:F:395:LYS:NZ	4:F:710:HOH:O	2.44	0.50
1:G:220:MET:HB3	1:G:367:VAL:HG21	1.93	0.50
1:E:211:GLU:OE1	4:E:702:HOH:O	2.20	0.50
1:C:10:GLN:HG3	1:C:23:PRO:HG2	1.94	0.50
1:B:104:GLU:OE1	1:B:290:ARG:NH2	2.44	0.50
1:H:187:ASP:OD2	1:H:189:ARG:NH2	2.41	0.50
1:F:140:PHE:CZ	1:F:231:ILE:HD11	2.47	0.49
1:B:419:ARG:O	1:B:422:GLN:HG2	2.12	0.49
1:C:170:PRO:HD3	4:C:704:HOH:O	2.12	0.49
1:B:77:HIS:HA	1:B:314:PRO:HD2	1.95	0.49
1:A:419:ARG:NH1	4:A:714:HOH:O	2.45	0.49
1:G:89:ILE:HD13	1:H:5:ASP:HB3	1.93	0.49
1:H:27:TYR:CE2	1:H:384:VAL:HG21	2.47	0.49
1:C:219:GLY:HA2	1:C:396:LEU:HD11	1.95	0.49
1:E:149:PHE:CZ	1:F:121:LYS:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:PHE:HZ	1:F:231:ILE:HD11	1.76	0.49
1:G:77:HIS:HA	1:G:314:PRO:HD2	1.95	0.49
1:G:245:ASP:HA	1:G:271:CYS:HB2	1.95	0.49
1:H:418:ASN:O	1:H:422:GLN:HG2	2.13	0.49
1:H:219:GLY:HA2	1:H:396:LEU:HD11	1.94	0.48
1:A:21:THR:HG22	1:B:294:GLU:HG2	1.95	0.48
1:G:110:ASP:HB3	1:H:282:THR:HG21	1.95	0.48
1:E:85:HIS:CD2	1:E:88:ALA:H	2.32	0.48
1:E:85:HIS:HD2	1:E:88:ALA:H	1.61	0.48
1:F:217:ALA:HB1	3:F:602:J4J:C25	2.44	0.48
2:D:601:PLP:O3P	4:D:701:HOH:O	2.20	0.48
1:A:165:TRP:CH2	1:B:121:LYS:HG3	2.48	0.48
1:E:21:THR:HG22	1:F:294:GLU:HG2	1.95	0.48
1:A:85:HIS:HE1	4:A:732:HOH:O	1.96	0.48
1:G:306:HIS:HD2	1:G:308:PRO:HD3	1.78	0.48
1:F:85:HIS:CE1	1:F:314:PRO:HG3	2.49	0.48
1:G:8:PHE:CZ	1:H:93:ARG:HA	2.48	0.48
4:C:704:HOH:O	1:D:170:PRO:HD3	2.14	0.48
1:F:370:THR:HG21	1:F:427:PHE:CE1	2.49	0.48
1:D:184:GLY:O	1:D:224:HIS:HD2	1.96	0.47
1:B:348:ALA:HA	1:B:351:ARG:NH1	2.29	0.47
1:G:36:GLU:HA	1:G:45:LEU:O	2.14	0.47
1:G:149:PHE:CZ	1:H:121:LYS:HG3	2.49	0.47
1:A:53:TRP:HB2	1:A:274:LYS:HD3	1.96	0.47
1:B:86:ALA:HB3	1:B:87:PRO:HD3	1.96	0.47
1:G:290:ARG:NH1	1:H:11:ARG:O	2.47	0.47
1:A:149:PHE:HA	1:A:152:MET:HE3	1.97	0.47
1:A:69:LYS:HG2	1:B:69:LYS:HG2	1.97	0.47
1:B:139:THR:OG1	1:B:140:PHE:N	2.48	0.47
1:F:418:ASN:O	1:F:422:GLN:HG2	2.15	0.47
1:G:127:TRP:CD2	1:G:134:ARG:HD2	2.50	0.47
1:G:274:LYS:HZ1	3:G:603:J4J:C18	2.27	0.47
1:C:164:LEU:N	4:C:701:HOH:O	2.44	0.46
1:F:132:GLU:O	1:F:134:ARG:N	2.40	0.46
1:B:370:THR:HG21	1:B:427:PHE:CE1	2.49	0.46
1:B:198:MET:O	1:B:202:ARG:N	2.49	0.46
1:E:36:GLU:HA	1:E:45:LEU:O	2.15	0.46
1:A:251:PHE:CE1	1:A:324:LEU:HD21	2.51	0.46
1:G:127:TRP:CE2	1:G:134:ARG:HD2	2.50	0.46
1:E:139:THR:OG1	1:E:140:PHE:N	2.49	0.46
1:C:127:TRP:CE2	1:C:134:ARG:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:TRP:CE3	1:D:226:GLU:HB3	2.51	0.46
1:H:147:ASP:OD2	3:H:603:J4J:N16	2.48	0.46
1:G:138:LEU:HB3	1:G:208:VAL:HG22	1.97	0.46
1:G:188:GLU:CD	1:G:230:ARG:HH12	2.18	0.45
1:F:2:THR:HG22	1:F:3:THR:H	1.81	0.45
1:C:202:ARG:HG3	1:C:203:HIS:CE1	2.52	0.45
1:F:370:THR:HG21	1:F:427:PHE:HE1	1.82	0.45
1:G:15:HIS:HB2	1:G:18:THR:HG21	1.99	0.45
1:G:305:MET:HE1	1:H:161:MET:HB2	1.99	0.45
1:A:53:TRP:N	1:A:400:MET:HE3	2.32	0.45
1:A:188:GLU:HG3	4:A:733:HOH:O	2.16	0.45
1:A:380:GLN:OE1	1:A:391:ARG:NH1	2.43	0.45
1:B:180:SER:N	1:B:190:ASP:OD2	2.34	0.45
1:B:230:ARG:O	1:B:234:ILE:HG13	2.17	0.45
1:D:380:GLN:OE1	1:D:391:ARG:HD2	2.16	0.45
1:G:127:TRP:CE3	1:G:130:LYS:HD3	2.52	0.45
1:B:251:PHE:CE1	1:B:324:LEU:HD21	2.52	0.45
1:F:382:PHE:O	1:F:386:GLN:HG2	2.16	0.45
1:H:253:ARG:HG3	1:H:365:ILE:HD11	1.98	0.45
1:E:246:GLU:HG3	1:E:270:LEU:HD11	1.98	0.45
1:A:199:ALA:HA	1:A:202:ARG:HD3	1.98	0.45
1:C:221:ARG:NH2	4:C:715:HOH:O	2.49	0.45
1:F:127:TRP:CE2	1:F:134:ARG:HD2	2.52	0.45
1:C:28:PRO:HG2	1:C:40:SER:HB2	1.99	0.44
1:E:110:ASP:OD2	1:E:110:ASP:N	2.46	0.44
1:H:357:ALA:HB2	1:H:371:THR:HG22	2.00	0.44
1:A:186:TRP:CE3	1:A:226:GLU:HB3	2.53	0.44
1:H:52:TRP:CD2	3:H:602:J4J:S21	3.10	0.44
1:C:82:GLY:HA2	1:D:26:VAL:HG12	1.99	0.44
1:C:202:ARG:HG3	1:C:203:HIS:ND1	2.32	0.44
1:G:201:HIS:O	1:G:204:GLU:HG2	2.18	0.44
1:E:106:VAL:HG22	1:E:287:LEU:HG	2.00	0.44
1:F:423:ASP:HA	4:F:773:HOH:O	2.17	0.44
1:E:217:ALA:HB1	3:E:602:J4J:C25	2.48	0.44
1:E:391:ARG:HE	3:E:603:J4J:C25	2.30	0.44
1:H:186:TRP:HZ3	1:H:227:TRP:CD1	2.36	0.44
1:H:243:ILE:HG12	1:H:269:ILE:HB	1.98	0.44
1:G:13:ILE:HD11	1:H:89:ILE:HA	1.99	0.44
1:C:15:HIS:HB2	1:C:18:THR:HG21	2.00	0.44
1:F:139:THR:OG1	1:F:140:PHE:N	2.51	0.44
1:C:108:LEU:O	1:C:311:MET:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:TRP:HB2	1:C:274:LYS:HD3	2.00	0.43
2:E:601:PLP:O3P	1:F:308:PRO:HA	2.18	0.43
1:G:201:HIS:ND1	1:G:204:GLU:OE2	2.38	0.43
1:H:85:HIS:CE1	1:H:314:PRO:HG3	2.53	0.43
1:B:156:ASP:HA	1:B:157:PRO:HD3	1.69	0.43
1:D:132:GLU:O	1:D:134:ARG:N	2.45	0.43
1:D:219:GLY:HA2	1:D:396:LEU:HD11	2.01	0.43
1:G:186:TRP:HZ3	1:G:227:TRP:CD1	2.37	0.43
1:D:104:GLU:OE1	1:D:290:ARG:NH2	2.47	0.43
1:E:340:GLU:HG2	1:E:344:ARG:NH1	2.33	0.43
1:G:121:LYS:HG3	1:H:165:TRP:CH2	2.54	0.43
1:A:408:GLN:HA	4:A:814:HOH:O	2.18	0.43
1:C:118:VAL:HG13	1:C:304:PHE:CE2	2.54	0.43
1:D:102:PRO:O	1:D:289:THR:HA	2.19	0.43
1:F:246:GLU:HG3	1:F:270:LEU:CD1	2.49	0.43
1:C:149:PHE:HD2	1:D:150:GLY:HA3	1.84	0.43
1:C:182:MET:HG3	1:C:183:ASP:CB	2.48	0.43
1:C:182:MET:HA	1:C:183:ASP:HA	1.74	0.43
1:A:121:LYS:HG3	1:B:149:PHE:CZ	2.54	0.43
1:C:348:ALA:N	1:C:349:PRO:HD2	2.33	0.43
1:E:19:SER:HB2	1:F:302:GLY:O	2.19	0.43
1:F:36:GLU:HA	1:F:45:LEU:O	2.18	0.43
1:F:380:GLN:OE1	1:F:391:ARG:HD2	2.18	0.43
1:G:134:ARG:HD3	1:G:205:ILE:O	2.19	0.43
1:H:334:GLN:NE2	1:H:338:ASP:OD1	2.47	0.43
1:B:140:PHE:CZ	1:B:231:ILE:HD11	2.53	0.43
1:C:245:ASP:HA	1:C:271:CYS:HB2	2.00	0.43
1:D:217:ALA:HB1	3:D:602:J4J:C25	2.48	0.43
1:A:77:HIS:HA	1:A:314:PRO:HD2	2.00	0.43
1:B:340:GLU:HG2	1:B:344:ARG:NH1	2.34	0.43
1:G:188:GLU:OE2	1:G:230:ARG:NH1	2.48	0.43
1:A:156:ASP:HA	1:A:157:PRO:HD3	1.90	0.42
1:C:116:VAL:HG21	1:C:145:HIS:HB3	2.00	0.42
1:E:24:LEU:HD21	1:H:429:GLN:HB3	2.00	0.42
1:E:33:GLU:OE2	1:E:44:ARG:NH2	2.45	0.42
1:E:245:ASP:HA	1:E:271:CYS:HB2	2.00	0.42
1:F:210:ILE:HA	4:F:751:HOH:O	2.19	0.42
1:H:359:VAL:HG22	1:H:368:VAL:HG22	2.01	0.42
1:C:10:GLN:HG3	1:C:23:PRO:CG	2.49	0.42
1:C:257:LEU:HA	1:C:257:LEU:HD12	1.76	0.42
1:D:80:PHE:HB2	1:D:311:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:HIS:ND1	1:E:204:GLU:OE2	2.42	0.42
1:H:27:TYR:CD1	1:H:27:TYR:N	2.88	0.42
1:E:108:LEU:O	1:E:311:MET:HG3	2.20	0.42
1:F:2:THR:HG22	1:F:3:THR:N	2.35	0.42
1:B:194:PHE:N	4:B:707:HOH:O	2.40	0.42
1:F:108:LEU:O	1:F:311:MET:HG3	2.19	0.42
1:H:230:ARG:NH1	4:H:702:HOH:O	2.29	0.42
1:A:36:GLU:HA	1:A:45:LEU:O	2.19	0.42
1:F:9:ASP:HA	1:F:13:ILE:HD12	2.02	0.42
1:G:412:ARG:NH1	4:G:705:HOH:O	2.30	0.42
1:H:246:GLU:OE1	1:H:249:THR:OG1	2.24	0.42
1:B:36:GLU:HA	1:B:45:LEU:O	2.20	0.42
1:E:342:GLN:NE2	1:E:410:LEU:HB3	2.34	0.42
1:F:312:GLY:O	1:F:313:ASN:C	2.58	0.42
1:G:116:VAL:O	1:G:120:MET:HG3	2.20	0.42
1:E:156:ASP:HA	1:E:157:PRO:HD3	1.80	0.41
1:A:105:CYS:O	1:A:287:LEU:HA	2.21	0.41
1:D:9:ASP:HA	1:D:13:ILE:HD12	2.02	0.41
1:E:10:GLN:HG3	1:E:23:PRO:HG2	2.02	0.41
1:G:382:PHE:O	1:G:386:GLN:HG2	2.20	0.41
1:D:53:TRP:HB2	1:D:274:LYS:HD3	2.01	0.41
1:E:109:ALA:O	1:E:283:LEU:HD12	2.20	0.41
1:F:183:ASP:OD2	1:F:184:GLY:N	2.50	0.41
1:G:108:LEU:O	1:G:311:MET:HG3	2.21	0.41
1:C:413:LEU:O	1:C:417:VAL:HG23	2.21	0.41
1:D:229:LYS:HG3	1:D:263:ALA:HB1	2.02	0.41
1:F:127:TRP:HB3	1:F:132:GLU:O	2.21	0.41
1:G:370:THR:HG21	1:G:427:PHE:HE1	1.84	0.41
1:B:186:TRP:CE3	1:B:226:GLU:HB3	2.55	0.41
1:C:118:VAL:HG13	1:C:304:PHE:CZ	2.54	0.41
1:D:230:ARG:HD3	4:D:703:HOH:O	2.19	0.41
1:G:325:ALA:O	1:G:328:GLU:HB2	2.21	0.41
1:D:423:ASP:CG	1:D:425:THR:HG1	2.24	0.41
1:F:14:TRP:CZ3	1:F:20:MET:HG2	2.55	0.41
1:F:344:ARG:HD2	4:F:789:HOH:O	2.21	0.41
1:B:132:GLU:O	1:B:134:ARG:N	2.48	0.41
1:B:224:HIS:HA	1:B:225:PRO:HD3	1.94	0.41
1:D:176:PRO:HB2	4:D:776:HOH:O	2.21	0.41
1:G:374:VAL:HG21	1:G:392:PRO:HB2	2.02	0.41
1:H:47:ASP:OD2	1:H:59:TYR:OH	2.28	0.41
1:A:90:GLU:OE2	1:A:94:LYS:NZ	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:TRP:HB3	1:B:132:GLU:O	2.20	0.41
1:C:149:PHE:CZ	1:D:121:LYS:HG3	2.55	0.41
1:C:251:PHE:CE1	1:C:324:LEU:HD21	2.56	0.41
1:E:5:ASP:HB3	1:F:89:ILE:HD13	2.03	0.41
1:G:162:HIS:O	1:G:166:LYS:N	2.51	0.41
1:H:77:HIS:HA	1:H:314:PRO:HD2	2.02	0.41
1:A:127:TRP:CE2	1:A:134:ARG:HD2	2.55	0.41
1:E:302:GLY:O	1:F:19:SER:HB2	2.21	0.41
1:G:368:VAL:HG11	1:G:421:VAL:HG21	2.03	0.41
1:H:127:TRP:CD2	1:H:134:ARG:HD2	2.56	0.41
1:A:39:LEU:HD12	1:A:43:ARG:HD2	2.02	0.40
1:A:370:THR:HG21	1:A:427:PHE:CE1	2.56	0.40
1:B:380:GLN:OE1	1:B:391:ARG:HD2	2.22	0.40
1:C:132:GLU:O	1:C:134:ARG:N	2.47	0.40
1:C:220:MET:HB3	1:C:367:VAL:HG21	2.03	0.40
1:D:123:ALA:HA	1:D:241:LEU:HD12	2.03	0.40
1:F:156:ASP:HA	1:F:157:PRO:HD3	1.82	0.40
1:C:36:GLU:HA	1:C:45:LEU:O	2.21	0.40
1:D:27:TYR:OH	1:D:381:LYS:HA	2.21	0.40
1:E:370:THR:HG21	1:E:427:PHE:CE1	2.56	0.40
1:B:106:VAL:HG22	1:B:287:LEU:HG	2.04	0.40
1:C:33:GLU:OE2	1:C:44:ARG:NH2	2.55	0.40
1:C:94:LYS:HE3	1:C:328:GLU:OE2	2.20	0.40
1:G:11:ARG:HB3	1:G:12:HIS:CD2	2.56	0.40
1:H:35:CYS:SG	1:H:404:ILE:HG13	2.62	0.40
1:H:423:ASP:OD1	1:H:424:GLU:N	2.51	0.40
1:C:6:LEU:HA	1:C:6:LEU:HD23	1.91	0.40
1:C:86:ALA:HB3	1:C:87:PRO:HD3	2.02	0.40
1:D:27:TYR:CD1	1:D:27:TYR:N	2.90	0.40
1:G:197:LEU:HA	1:G:197:LEU:HD23	1.90	0.40
4:G:701:HOH:O	1:H:288:THR:HG22	2.21	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	427/429 (100%)	410 (96%)	14 (3%)	3 (1%)	22	26
1	B	427/429 (100%)	411 (96%)	14 (3%)	2 (0%)	29	34
1	C	427/429 (100%)	409 (96%)	15 (4%)	3 (1%)	22	26
1	D	427/429 (100%)	410 (96%)	15 (4%)	2 (0%)	29	34
1	E	427/429 (100%)	408 (96%)	16 (4%)	3 (1%)	22	26
1	F	427/429 (100%)	410 (96%)	13 (3%)	4 (1%)	17	20
1	G	427/429 (100%)	412 (96%)	13 (3%)	2 (0%)	29	34
1	H	427/429 (100%)	413 (97%)	12 (3%)	2 (0%)	29	34
All	All	3416/3432 (100%)	3283 (96%)	112 (3%)	21 (1%)	25	29

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	ALA
1	B	133	ALA
1	C	133	ALA
1	D	133	ALA
1	E	184	GLY
1	F	133	ALA
1	F	184	GLY
1	F	274	LYS
1	H	166	LYS
1	A	274	LYS
1	E	274	LYS
1	G	274	LYS
1	D	166	LYS
1	A	307	GLY
1	G	307	GLY
1	B	307	GLY
1	C	216	GLY
1	C	307	GLY
1	E	307	GLY
1	F	307	GLY
1	H	307	GLY

### 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	334/344 (97%)	327 (98%)	7 (2%)	53	66
1	B	337/344 (98%)	332 (98%)	5 (2%)	65	76
1	C	325/344 (94%)	319 (98%)	6 (2%)	59	71
1	D	336/344 (98%)	334 (99%)	2 (1%)	86	91
1	E	329/344 (96%)	326 (99%)	3 (1%)	78	87
1	F	329/344 (96%)	326 (99%)	3 (1%)	78	87
1	G	321/344 (93%)	318 (99%)	3 (1%)	78	87
1	H	331/344 (96%)	327 (99%)	4 (1%)	71	81
All	All	2642/2752 (96%)	2609 (99%)	33 (1%)	71	81

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	14	TRP
1	A	18	THR
1	A	110	ASP
1	A	132	GLU
1	A	290	ARG
1	A	419	ARG
1	B	3	THR
1	B	14	TRP
1	B	60	ASN
1	B	110	ASP
1	B	421	VAL
1	C	2	THR
1	C	14	TRP
1	C	40	SER
1	C	80	PHE
1	C	110	ASP
1	C	265	ILE
1	D	18	THR

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Mol	Chain	Res	Type
1	D	110	ASP
1	E	60	ASN
1	E	110	ASP
1	E	410	LEU
1	F	110	ASP
1	F	210	ILE
1	F	265	ILE
1	G	11	ARG
1	G	110	ASP
1	G	421	VAL
1	H	80	PHE
1	H	110	ASP
1	H	192	VAL
1	H	290	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	372	HIS
1	C	203	HIS
1	C	386	GLN
1	E	85	HIS
1	E	128	GLN
1	F	429	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	J4J	C	603	-	14,15,15	2.15	2 (14%)	15,19,19	3.08	3 (20%)
2	PLP	B	601	3	15,15,16	1.00	1 (6%)	20,22,23	1.09	0
2	PLP	G	601	3	15,15,16	1.04	1 (6%)	20,22,23	1.49	4 (20%)
3	J4J	F	602	2	14,15,15	2.20	3 (21%)	15,19,19	1.58	2 (13%)
3	J4J	E	602	2	14,15,15	2.43	3 (21%)	15,19,19	1.62	1 (6%)
2	PLP	E	601	3	15,15,16	1.01	1 (6%)	20,22,23	1.56	4 (20%)
3	J4J	A	602	2	14,15,15	2.17	3 (21%)	15,19,19	1.61	2 (13%)
3	J4J	D	602	2	14,15,15	2.26	3 (21%)	15,19,19	1.51	2 (13%)
3	J4J	B	603	-	13,14,15	1.80	2 (15%)	15,17,19	2.22	5 (33%)
3	J4J	H	603	-	14,15,15	2.03	2 (14%)	15,19,19	1.82	4 (26%)
2	PLP	F	601	3	15,15,16	0.96	0	20,22,23	1.74	3 (15%)
3	J4J	F	603	-	14,15,15	2.29	2 (14%)	15,19,19	2.42	3 (20%)
3	J4J	G	602	-	14,15,15	2.11	3 (21%)	15,19,19	1.37	3 (20%)
2	PLP	A	601	3	15,15,16	0.78	0	20,22,23	1.16	1 (5%)
3	J4J	D	603	-	14,15,15	1.98	2 (14%)	15,19,19	2.80	5 (33%)
3	J4J	H	602	2	14,15,15	2.34	3 (21%)	15,19,19	4.55	5 (33%)
2	PLP	D	601	3	15,15,16	1.07	1 (6%)	20,22,23	1.25	2 (10%)
3	J4J	G	603	2	14,15,15	2.16	3 (21%)	15,19,19	2.10	3 (20%)
2	PLP	H	601	3	15,15,16	1.14	2 (13%)	20,22,23	1.16	2 (10%)
2	PLP	C	601	3	15,15,16	0.76	0	20,22,23	1.45	3 (15%)
3	J4J	E	603	-	14,15,15	2.05	3 (21%)	15,19,19	2.19	3 (20%)
3	J4J	A	603	-	14,15,15	2.06	3 (21%)	15,19,19	1.96	3 (20%)
3	J4J	C	602	2	14,15,15	2.12	3 (21%)	15,19,19	1.10	1 (6%)
3	J4J	B	602	2	14,15,15	2.15	3 (21%)	15,19,19	1.24	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	J4J	C	603	-	-	2/9/11/11	0/1/1/1
2	PLP	B	601	3	-	0/6/6/8	0/1/1/1
2	PLP	G	601	3	-	0/6/6/8	0/1/1/1
3	J4J	F	602	2	-	2/9/11/11	0/1/1/1
3	J4J	E	602	2	-	3/9/11/11	0/1/1/1
2	PLP	E	601	3	-	2/6/6/8	0/1/1/1
3	J4J	A	602	2	-	2/9/11/11	0/1/1/1
3	J4J	D	602	2	-	4/9/11/11	0/1/1/1
3	J4J	B	603	-	-	1/7/9/11	0/1/1/1
3	J4J	H	603	-	-	2/9/11/11	0/1/1/1
2	PLP	F	601	3	-	0/6/6/8	0/1/1/1
3	J4J	F	603	-	-	2/9/11/11	0/1/1/1
3	J4J	G	602	-	-	4/9/11/11	0/1/1/1
2	PLP	A	601	3	-	0/6/6/8	0/1/1/1
3	J4J	D	603	-	-	0/9/11/11	0/1/1/1
3	J4J	H	602	2	-	4/9/11/11	0/1/1/1
2	PLP	D	601	3	-	0/6/6/8	0/1/1/1
3	J4J	G	603	2	-	2/9/11/11	0/1/1/1
2	PLP	H	601	3	-	0/6/6/8	0/1/1/1
2	PLP	C	601	3	-	0/6/6/8	0/1/1/1
3	J4J	E	603	-	-	3/9/11/11	0/1/1/1
3	J4J	A	603	-	-	2/9/11/11	0/1/1/1
3	J4J	C	602	2	-	4/9/11/11	0/1/1/1
3	J4J	B	602	2	-	4/9/11/11	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	603	J4J	N16-N17	-6.72	1.31	1.41
3	E	602	J4J	N16-N17	-6.67	1.31	1.41
3	H	602	J4J	N16-N17	-6.61	1.31	1.41
3	F	602	J4J	N16-N17	-6.39	1.32	1.41
3	A	602	J4J	N16-N17	-6.15	1.32	1.41
3	D	602	J4J	N16-N17	-6.13	1.32	1.41
3	H	603	J4J	N16-N17	-6.04	1.32	1.41
3	A	603	J4J	N16-N17	-6.03	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	J4J	N16-N17	-6.01	1.32	1.41
3	G	603	J4J	N16-N17	-6.00	1.32	1.41
3	G	602	J4J	N16-N17	-5.82	1.33	1.41
3	D	603	J4J	N16-N17	-5.79	1.33	1.41
3	B	603	J4J	N16-N17	-5.78	1.33	1.41
3	E	603	J4J	N16-N17	-5.58	1.33	1.41
3	C	602	J4J	N16-N17	-5.40	1.33	1.41
3	B	602	J4J	N16-N17	-5.34	1.33	1.41
3	E	602	J4J	C22-S21	-5.24	1.69	1.77
3	B	602	J4J	C22-S21	-4.78	1.70	1.77
3	C	603	J4J	C22-S21	-4.70	1.70	1.77
3	D	602	J4J	C22-S21	-4.70	1.70	1.77
3	F	603	J4J	C22-S21	-4.63	1.70	1.77
3	G	603	J4J	C22-S21	-4.49	1.70	1.77
3	G	602	J4J	C22-S21	-4.33	1.70	1.77
3	H	602	J4J	C22-S21	-4.29	1.70	1.77
3	F	602	J4J	C22-S21	-4.21	1.71	1.77
3	H	603	J4J	C22-S21	-4.13	1.71	1.77
3	E	603	J4J	C22-S21	-4.08	1.71	1.77
3	A	602	J4J	C22-S21	-4.02	1.71	1.77
3	A	603	J4J	C22-S21	-3.92	1.71	1.77
3	C	602	J4J	C22-S21	-3.76	1.71	1.77
3	C	602	J4J	C27-N28	-3.58	1.39	1.45
3	D	603	J4J	C22-S21	-3.53	1.72	1.77
2	H	601	PLP	C3-C2	-3.11	1.37	1.40
3	B	602	J4J	C27-N28	-3.09	1.40	1.45
2	D	601	PLP	C3-C2	-2.96	1.37	1.40
3	A	602	J4J	C27-N28	-2.93	1.40	1.45
3	D	602	J4J	C27-N28	-2.78	1.40	1.45
2	E	601	PLP	C3-C2	-2.78	1.38	1.40
3	E	603	J4J	C27-N28	-2.71	1.40	1.45
3	G	602	J4J	C27-N28	-2.67	1.40	1.45
3	E	602	J4J	C27-N28	-2.65	1.40	1.45
2	G	601	PLP	C3-C2	-2.61	1.38	1.40
3	H	602	J4J	C27-N28	-2.59	1.41	1.45
3	B	603	J4J	C22-S21	-2.50	1.73	1.77
3	A	603	J4J	C27-N28	-2.35	1.41	1.45
2	B	601	PLP	C3-C2	-2.24	1.38	1.40
3	F	602	J4J	C27-N28	-2.23	1.41	1.45
3	G	603	J4J	C27-N28	-2.11	1.41	1.45
2	H	601	PLP	C4A-C4	-2.09	1.47	1.51

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	602	J4J	C20-S21-C22	15.28	126.07	102.61
3	C	603	J4J	C20-S21-C22	10.42	118.60	102.61
3	F	603	J4J	C20-S21-C22	8.41	115.51	102.61
3	D	603	J4J	C20-S21-C22	8.26	115.29	102.61
3	E	603	J4J	C20-S21-C22	7.34	113.89	102.61
3	G	603	J4J	C20-S21-C22	6.22	112.16	102.61
3	A	603	J4J	C20-S21-C22	5.90	111.67	102.61
3	B	603	J4J	C20-S21-C22	5.90	111.67	102.61
3	E	602	J4J	C20-S21-C22	5.46	111.00	102.61
3	H	602	J4J	C23-C22-S21	-4.95	109.38	121.46
3	F	602	J4J	C20-S21-C22	4.91	110.15	102.61
3	H	602	J4J	C27-C22-S21	4.71	130.86	120.52
3	H	603	J4J	C20-S21-C22	4.69	109.81	102.61
3	A	602	J4J	C20-S21-C22	4.63	109.72	102.61
3	D	602	J4J	C20-S21-C22	4.54	109.58	102.61
3	B	602	J4J	C20-S21-C22	3.98	108.72	102.61
2	F	601	PLP	C4A-C4-C5	-3.94	116.88	120.94
3	G	603	J4J	C26-C27-N28	3.65	120.38	116.47
2	E	601	PLP	O4P-C5A-C5	3.56	116.14	109.35
3	D	603	J4J	C18-N17-N16	-3.49	114.84	122.08
3	C	603	J4J	C23-C22-S21	-3.47	113.00	121.46
3	G	602	J4J	C20-S21-C22	3.37	107.79	102.61
3	A	602	J4J	C26-C27-N28	3.31	120.01	116.47
3	H	602	J4J	C26-C27-N28	-3.28	112.97	116.47
2	F	601	PLP	C6-C5-C4	3.23	120.70	118.16
2	C	601	PLP	C6-C5-C4	3.22	120.69	118.16
3	D	603	J4J	C26-C27-N28	-3.04	113.23	116.47
3	B	603	J4J	C18-N17-N16	-3.02	115.83	122.08
2	F	601	PLP	C5-C6-N1	-3.02	118.79	123.82
2	G	601	PLP	O4P-C5A-C5	2.96	114.98	109.35
3	D	603	J4J	C23-C22-S21	-2.90	114.39	121.46
2	C	601	PLP	O2P-P-O4P	-2.89	99.03	106.73
3	D	602	J4J	C26-C27-N28	2.89	119.56	116.47
3	C	603	J4J	C27-C22-S21	2.85	126.77	120.52
2	E	601	PLP	O3P-P-O4P	-2.81	99.27	106.73
2	G	601	PLP	C4A-C4-C5	-2.76	118.09	120.94
3	B	603	J4J	C22-C27-N28	2.65	122.19	120.14
3	H	603	J4J	C18-N17-N16	-2.62	116.66	122.08
3	D	603	J4J	C27-C22-S21	2.59	126.21	120.52
3	F	602	J4J	C26-C27-N28	2.46	119.10	116.47
3	C	602	J4J	C26-C27-N28	2.45	119.09	116.47
3	B	603	J4J	C23-C22-C27	-2.45	116.76	119.49
2	D	601	PLP	O3P-P-O4P	-2.30	100.61	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	PLP	O3P-P-O2P	2.27	116.31	107.64
3	G	602	J4J	C23-C22-S21	-2.26	115.94	121.46
3	F	603	J4J	C26-C27-N28	2.24	118.87	116.47
2	G	601	PLP	O2P-P-O4P	-2.23	100.80	106.73
3	A	603	J4J	C27-C22-S21	2.21	125.38	120.52
2	G	601	PLP	C5-C6-N1	-2.20	120.16	123.82
3	H	603	J4J	C26-C27-N28	2.17	118.79	116.47
3	F	603	J4J	C18-N17-N16	-2.16	117.60	122.08
2	A	601	PLP	O3P-P-O2P	2.15	115.84	107.64
3	A	603	J4J	C23-C22-S21	-2.14	116.24	121.46
3	G	602	J4J	C27-C22-S21	2.14	125.21	120.52
3	H	602	J4J	C25-C24-C23	-2.13	116.94	120.19
3	B	603	J4J	C24-C23-C22	2.13	123.33	119.63
3	E	603	J4J	C23-C22-S21	-2.10	116.35	121.46
2	C	601	PLP	O3P-P-O2P	2.10	115.64	107.64
2	E	601	PLP	C5A-C5-C6	-2.09	115.94	119.37
3	H	603	J4J	C23-C22-S21	-2.07	116.41	121.46
2	E	601	PLP	C2A-C2-N1	2.07	121.71	117.67
2	H	601	PLP	O3P-P-O4P	-2.06	101.26	106.73
2	D	601	PLP	C5-C6-N1	-2.04	120.42	123.82
3	G	603	J4J	C18-N17-N16	2.01	126.24	122.08
3	E	603	J4J	C18-N17-N16	-2.00	117.94	122.08

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	601	PLP	C4-C5-C5A-O4P
2	E	601	PLP	C6-C5-C5A-O4P
3	A	602	J4J	C26-C27-N28-O30
3	A	602	J4J	C22-C27-N28-O30
3	A	603	J4J	C26-C27-N28-O30
3	A	603	J4J	C22-C27-N28-O30
3	C	602	J4J	C20-C18-N17-N16
3	C	602	J4J	O19-C18-N17-N16
3	C	603	J4J	C26-C27-N28-O30
3	C	603	J4J	C22-C27-N28-O30
3	D	602	J4J	C26-C27-N28-O30
3	E	602	J4J	C26-C27-N28-O30
3	E	602	J4J	C22-C27-N28-O30
3	E	603	J4J	C26-C27-N28-O30
3	E	603	J4J	C22-C27-N28-O30

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Mol	Chain	Res	Type	Atoms
3	F	602	J4J	C26-C27-N28-O30
3	F	602	J4J	C22-C27-N28-O30
3	F	603	J4J	C26-C27-N28-O30
3	F	603	J4J	C22-C27-N28-O30
3	G	602	J4J	C26-C27-N28-O30
3	G	602	J4J	C22-C27-N28-O30
3	H	602	J4J	C27-C22-S21-C20
3	H	602	J4J	C23-C22-S21-C20
3	B	602	J4J	C26-C27-N28-O30
3	C	602	J4J	C26-C27-N28-O30
3	G	603	J4J	C26-C27-N28-O30
3	H	603	J4J	C26-C27-N28-O30
3	B	602	J4J	O19-C18-N17-N16
3	H	602	J4J	O19-C18-N17-N16
3	D	602	J4J	C20-C18-N17-N16
3	E	602	J4J	C20-C18-N17-N16
3	B	603	J4J	C18-C20-S21-C22
3	G	602	J4J	C18-C20-S21-C22
3	D	602	J4J	O19-C18-N17-N16
3	B	602	J4J	C22-C27-N28-O30
3	C	602	J4J	C22-C27-N28-O30
3	D	602	J4J	C22-C27-N28-O30
3	G	603	J4J	C22-C27-N28-O30
3	H	603	J4J	C22-C27-N28-O30
3	B	602	J4J	C20-C18-N17-N16
3	H	602	J4J	C20-C18-N17-N16
3	E	603	J4J	C27-C22-S21-C20
3	G	602	J4J	C27-C22-S21-C20

There are no ring outliers.

17 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	J4J	1	0
3	F	602	J4J	1	0
3	E	602	J4J	1	0
2	E	601	PLP	2	0
3	A	602	J4J	1	0
3	D	602	J4J	1	0
3	H	603	J4J	2	0
3	F	603	J4J	1	0
3	G	602	J4J	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PLP	1	0
3	D	603	J4J	1	0
3	H	602	J4J	1	0
2	D	601	PLP	1	0
3	G	603	J4J	1	0
3	E	603	J4J	2	0
3	A	603	J4J	2	0
3	C	602	J4J	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	429/429 (100%)	-0.32	1 (0%) 95 95	10, 24, 49, 79	0
1	B	429/429 (100%)	-0.44	5 (1%) 79 77	10, 22, 46, 78	0
1	C	429/429 (100%)	-0.04	15 (3%) 44 40	15, 33, 67, 87	0
1	D	429/429 (100%)	-0.37	9 (2%) 63 60	13, 26, 50, 81	0
1	E	429/429 (100%)	-0.42	2 (0%) 91 91	13, 27, 49, 77	0
1	F	429/429 (100%)	-0.19	5 (1%) 79 77	15, 29, 50, 81	0
1	G	429/429 (100%)	0.15	21 (4%) 29 27	23, 44, 70, 87	0
1	H	429/429 (100%)	-0.19	7 (1%) 72 69	17, 34, 61, 83	0
All	All	3432/3432 (100%)	-0.23	65 (1%) 66 63	10, 30, 60, 87	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1	ALA	6.0
1	G	159	ASN	5.6
1	D	1	ALA	5.5
1	F	1	ALA	5.1
1	C	186	TRP	4.5
1	C	192	VAL	4.3
1	C	167	GLY	4.1
1	G	185	GLU	3.8
1	G	160	SER	3.7
1	G	193	GLY	3.6
1	B	133	ALA	3.5
1	D	163	SER	3.5
1	H	423	ASP	3.5
1	G	192	VAL	3.5
1	C	184	GLY	3.4
1	G	2	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	160	SER	3.3
1	D	162	HIS	3.2
1	C	235	CYS	3.0
1	G	352	ASP	3.0
1	G	197	LEU	3.0
1	G	353	ALA	3.0
1	G	3	THR	3.0
1	F	168	TYR	2.9
1	F	2	THR	2.8
1	C	199	ALA	2.8
1	G	346	GLN	2.7
1	B	163	SER	2.7
1	G	184	GLY	2.7
1	H	376	MET	2.7
1	H	283	LEU	2.7
1	H	426	PHE	2.6
1	G	356	VAL	2.6
1	C	183	ASP	2.6
1	C	162	HIS	2.6
1	E	133	ALA	2.5
1	C	197	LEU	2.5
1	C	356	VAL	2.5
1	E	160	SER	2.5
1	D	167	GLY	2.4
1	G	169	LEU	2.4
1	H	163	SER	2.4
1	G	186	TRP	2.4
1	G	235	CYS	2.4
1	B	160	SER	2.4
1	G	350	ALA	2.4
1	F	109	ALA	2.3
1	C	351	ARG	2.3
1	G	187	ASP	2.3
1	D	166	LYS	2.3
1	D	307	GLY	2.3
1	C	200	ALA	2.3
1	B	167	GLY	2.2
1	B	162	HIS	2.2
1	D	422	GLN	2.2
1	H	184	GLY	2.2
1	C	111	SER	2.2
1	C	166	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	308	PRO	2.1
1	D	189	ARG	2.1
1	F	115	ALA	2.1
1	G	351	ARG	2.1
1	G	354	GLU	2.1
1	C	300	GLU	2.0
1	H	310	PHE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	J4J	F	603	15/15	0.80	0.26	27,43,56,68	0
3	J4J	G	602	15/15	0.81	0.24	32,48,58,61	0
3	J4J	C	603	15/15	0.83	0.27	33,47,55,84	0
3	J4J	H	603	15/15	0.83	0.23	35,45,54,62	0
3	J4J	D	603	15/15	0.84	0.21	29,36,56,62	0
3	J4J	A	603	15/15	0.85	0.25	27,42,47,58	0
3	J4J	E	603	15/15	0.87	0.20	30,40,50,65	0
3	J4J	B	603	14/15	0.88	0.20	27,34,45,50	0
3	J4J	H	602	15/15	0.90	0.15	24,38,43,44	0
3	J4J	G	603	15/15	0.94	0.15	32,42,47,47	0
3	J4J	C	602	15/15	0.95	0.18	27,40,47,55	0
3	J4J	F	602	15/15	0.96	0.15	22,30,35,36	0
2	PLP	G	601	15/16	0.97	0.24	24,31,35,37	0
3	J4J	A	602	15/15	0.97	0.15	15,27,33,33	0
2	PLP	C	601	15/16	0.97	0.20	19,23,27,28	0
3	J4J	D	602	15/15	0.97	0.12	15,26,34,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	J4J	B	602	15/15	0.98	0.13	15,20,35,38	0
2	PLP	H	601	15/16	0.98	0.16	16,20,26,26	0
3	J4J	E	602	15/15	0.98	0.11	18,27,32,36	0
2	PLP	E	601	15/16	0.98	0.16	15,20,23,28	0
2	PLP	A	601	15/16	0.98	0.21	11,15,17,18	0
2	PLP	D	601	15/16	0.99	0.17	13,15,17,18	0
2	PLP	B	601	15/16	0.99	0.15	9,12,15,21	0
2	PLP	F	601	15/16	0.99	0.23	12,18,23,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.