



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:58 AM GMT

PDB ID : 1SO2  
Title : CATALYTIC DOMAIN OF HUMAN PHOSPHODIESTERASE 3B In COMPLEX WITH A DIHYDROPYRIDAZINE INHIBITOR  
Authors : Scapin, G.; Patel, S.B.; Chung, C.; Varnerin, J.P.; Edmondson, S.D.; Mastracchio, A.; Parmee, E.R.; Becker, J.W.; Singh, S.B.; Van Der Ploeg, L.H.; Tota, M.R.  
Deposited on : 2004-03-12  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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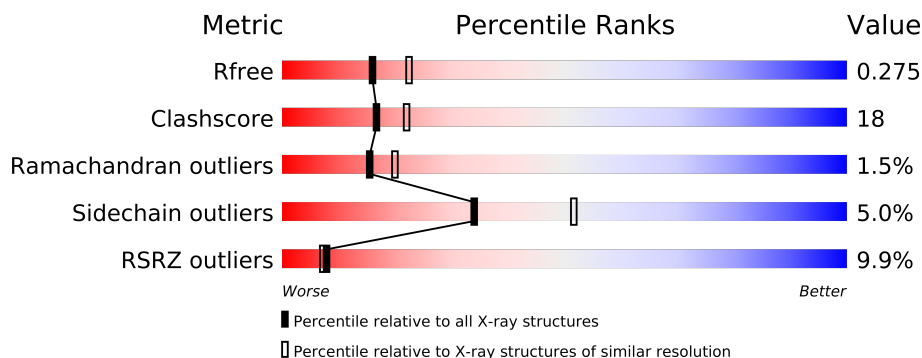
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	420	
1	B	420	
1	C	420	
1	D	420	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	HG9	A	453	-	X
3	HG9	B	451	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12292 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

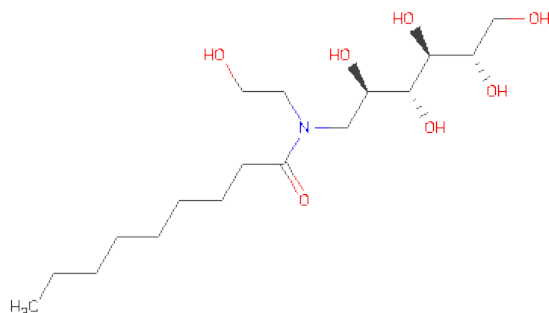
- Molecule 1 is a protein called cGMP-inhibited 3',5'-cyclic phosphodiesterase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2916	1868	501	533	14			
1	B	363	Total	C	N	O	S	0	0	0
			2909	1863	500	532	14			
1	C	372	Total	C	N	O	S	0	0	0
			2964	1897	508	545	14			
1	D	365	Total	C	N	O	S	0	0	0
			2916	1867	500	535	14			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

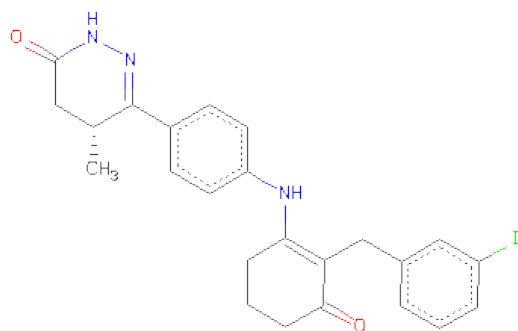
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	3	Total	Mg	0	0
			3	3		
2	D	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 1-DEOXY-1-[(2-HYDROXYETHYL)(NONANOYL)AMINO]HEXITOL (three-letter code: HG9) (formula: C<sub>17</sub>H<sub>35</sub>NO<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			24	16	1	7		
3	B	1	Total	C	N	O	0	0
			24	16	1	7		
3	A	1	Total	C	N	O	0	0
			24	16	1	7		
3	A	1	Total	C	N	O	0	0
			24	16	1	7		

- Molecule 4 is 6-(4-{[2-(3-iodobenzyl)-3-oxocyclohex-1-en-1-yl]amino}phenyl)-5-methyl-4,5-dihydropyridazin-3(2H)-one (three-letter code: 666) (formula: C<sub>24</sub>H<sub>24</sub>IN<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	I	N	O	0	0
			30	24	1	3	2		
4	B	1	Total	C	I	N	O	0	0
			30	24	1	3	2		
4	C	1	Total	C	I	N	O	0	0
			30	24	1	3	2		
4	D	1	Total	C	I	N	O	0	0
			30	24	1	3	2		

- Molecule 5 is water.

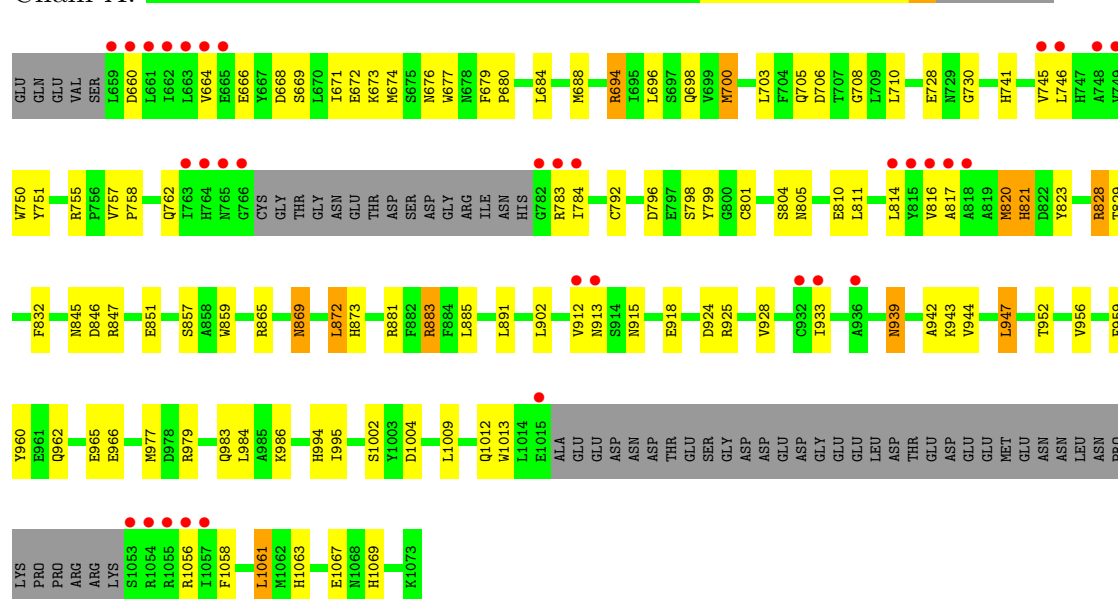
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	115	Total	O	0	0
			115	115		
5	C	70	Total	O	0	0
			70	70		
5	D	58	Total	O	0	0
			58	58		

### 3 Residue-property plots

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

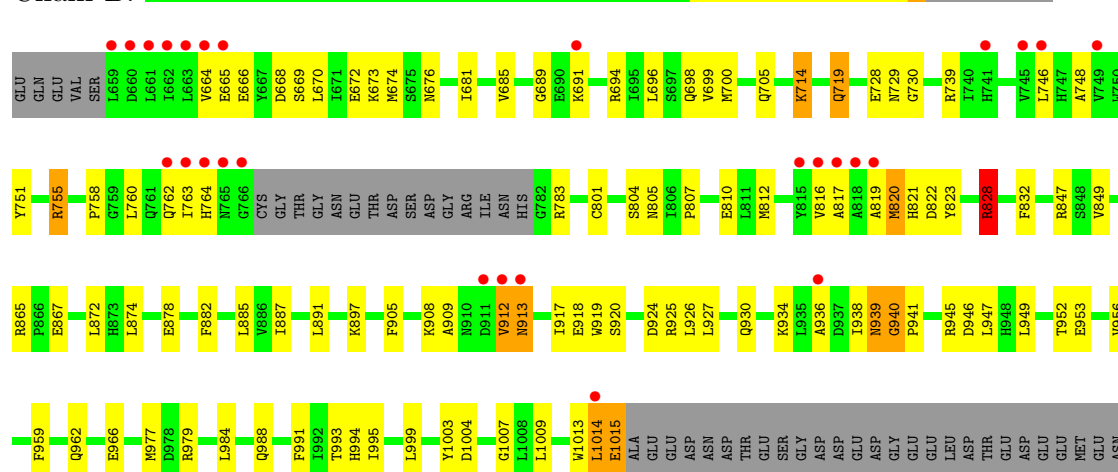
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

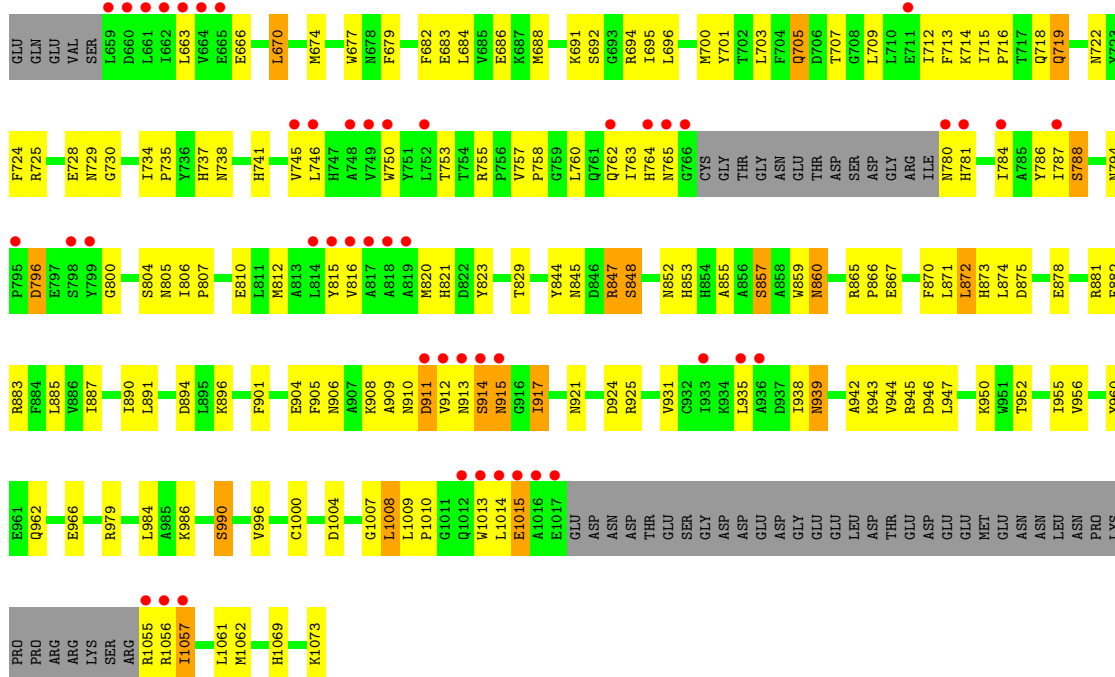
Chain A:



- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.48Å 121.77Å 126.67Å 90.00° 100.74° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.40) 99.8 (29.82-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 2.39Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.232 , 0.277 0.229 , 0.275	Depositor DCC
$R_{free}$ test set	4345 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.881	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 85711 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 666, MG, HG9

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	0.59	0/2992	0.67	1/4063 (0.0%)
1	B	0.58	0/2985	0.70	1/4054 (0.0%)
1	C	0.55	0/3040	0.66	0/4129
1	D	0.58	0/2992	0.64	0/4065
All	All	0.57	0/12009	0.67	2/16311 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	828	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	821	HIS	N-CA-C	5.22	125.09	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2916	0	2803	83	0
1	B	2909	0	2788	107	0
1	C	2964	0	2834	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2916	0	2788	148	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	48	0	60	2	0
3	B	48	0	60	2	0
4	A	30	0	24	2	0
4	B	30	0	24	2	0
4	C	30	0	24	1	0
4	D	30	0	24	3	0
5	A	119	0	0	2	0
5	B	115	0	0	6	0
5	C	70	0	0	3	0
5	D	58	0	0	4	0
All	All	12292	0	11429	419	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (419) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:700:MET:HE3	1:A:746:LEU:HD21	1.38	1.00
1:C:828:ARG:HG2	1:C:832:PHE:CD2	1.96	0.99
1:C:967:ALA:HB2	1:C:973:ILE:HD11	1.45	0.96
1:B:828:ARG:HG2	1:B:832:PHE:CD2	2.04	0.93
1:B:719:GLN:H	1:B:719:GLN:HE21	0.99	0.92
1:A:1061:LEU:HD23	1:A:1061:LEU:H	1.38	0.89
1:B:719:GLN:HE21	1:B:719:GLN:N	1.70	0.89
1:B:1014:LEU:H	1:B:1014:LEU:HD12	1.39	0.87
1:B:1009:LEU:HD22	1:B:1061:LEU:HD21	1.58	0.86
1:C:670:LEU:HD22	1:C:702:THR:HG21	1.58	0.86
1:C:994:HIS:O	1:C:995:ILE:HD13	1.76	0.85
1:D:679:PHE:HZ	1:D:684:LEU:HD22	1.41	0.84
1:A:828:ARG:HG2	1:A:832:PHE:CD2	2.15	0.81
1:B:939:ASN:HD22	1:B:939:ASN:C	1.83	0.81
1:A:939:ASN:C	1:A:939:ASN:HD22	1.85	0.80
1:B:700:MET:HE3	1:B:746:LEU:HD13	1.65	0.78
1:B:719:GLN:NE2	1:B:719:GLN:H	1.80	0.77
1:B:1015:GLU:HA	1:B:1015:GLU:OE1	1.85	0.75
1:D:872:LEU:HD13	1:D:873:HIS:CD2	2.22	0.75
1:D:716:PRO:HB2	1:D:719:GLN:HE22	1.53	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:847:ARG:CZ	1:B:891:LEU:HD13	2.17	0.73
1:C:730:GLY:HA3	1:C:823:TYR:CE1	2.23	0.73
1:C:751:TYR:CE2	1:C:755:ARG:HG3	2.24	0.73
1:B:905:PHE:HA	1:B:927:LEU:HD21	1.69	0.73
1:A:730:GLY:HA3	1:A:823:TYR:CE1	2.23	0.73
1:D:816:VAL:O	1:D:820:MET:HG2	1.89	0.73
1:B:1009:LEU:CD2	1:B:1061:LEU:HD21	2.20	0.72
1:D:956:VAL:HG11	1:D:984:LEU:HD13	1.69	0.72
1:B:909:ALA:HB2	1:B:917:ILE:HD11	1.70	0.72
1:D:921:ASN:HB3	1:D:924:ASP:HB2	1.72	0.72
1:B:991:PHE:HA	1:B:995:ILE:HD13	1.72	0.71
1:A:979:ARG:HH11	3:A:453:HG9:H602	1.53	0.71
1:C:828:ARG:HG2	1:C:832:PHE:CG	2.26	0.71
1:D:881:ARG:HG3	1:D:881:ARG:HH11	1.56	0.71
1:B:764:HIS:HB2	1:B:804:SER:O	1.90	0.71
1:B:995:ILE:N	1:B:995:ILE:HD12	2.07	0.70
1:D:716:PRO:HB2	1:D:719:GLN:NE2	2.06	0.70
1:A:762:GLN:NE2	1:A:801:CYS:H	1.90	0.70
4:C:463:666:H28	4:C:463:666:H162	1.72	0.69
1:D:688:MET:HE2	1:D:692:SER:HA	1.74	0.69
1:B:1014:LEU:N	1:B:1014:LEU:HD12	2.06	0.69
1:D:709:LEU:HD23	1:D:787:ILE:HD11	1.75	0.69
1:B:1069:HIS:NE2	1:B:1073:LYS:HD2	2.08	0.69
1:D:762:GLN:OE1	1:D:804:SER:HB2	1.93	0.69
1:D:784:ILE:HD12	1:D:807:PRO:HB3	1.74	0.68
1:B:1069:HIS:CD2	1:B:1073:LYS:HD2	2.29	0.67
1:D:935:LEU:HD11	1:D:1000:CYS:SG	2.34	0.67
1:D:865:ARG:HG2	1:D:865:ARG:HH11	1.59	0.67
1:C:912:VAL:HG23	1:C:913:ASN:N	2.10	0.67
1:D:718:GLN:HE21	1:D:722:ASN:HD21	1.41	0.67
1:A:883:ARG:HH11	1:A:883:ARG:HG2	1.59	0.67
1:D:700:MET:HE2	1:D:746:LEU:HD21	1.77	0.67
1:D:906:ASN:O	1:D:911:ASP:HB2	1.95	0.67
1:A:700:MET:HE3	1:A:746:LEU:CD2	2.20	0.66
1:D:1013:TRP:HA	1:D:1057:ILE:HG22	1.75	0.66
1:B:700:MET:HE3	1:B:746:LEU:CD1	2.25	0.66
1:A:939:ASN:C	1:A:939:ASN:ND2	2.46	0.66
1:C:763:ILE:HG13	1:C:764:HIS:N	2.10	0.66
1:D:1004:ASP:HB2	1:D:1009:LEU:HD12	1.77	0.66
1:D:725:ARG:O	1:D:729:ASN:ND2	2.29	0.66
1:D:763:ILE:C	1:D:765:ASN:H	2.00	0.66
1:C:960:TYR:HB3	1:C:979:ARG:NH2	2.11	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:962:GLN:O	1:C:966:GLU:HG3	1.96	0.65
1:A:816:VAL:O	1:A:820:MET:HG3	1.97	0.64
1:C:696:LEU:HB3	1:C:728:GLU:HG2	1.79	0.64
1:D:804:SER:C	1:D:805:ASN:HD22	2.00	0.64
1:A:1063:HIS:O	1:A:1067:GLU:HG3	1.98	0.64
1:D:912:VAL:C	1:D:914:SER:H	1.99	0.64
1:C:732:ARG:NH1	1:C:826:PRO:HA	2.12	0.63
1:A:1012:GLN:HE21	1:A:1058:PHE:HD2	1.45	0.63
1:D:853:HIS:O	1:D:857:SER:HB2	1.98	0.63
1:B:939:ASN:ND2	1:B:939:ASN:C	2.52	0.63
1:A:696:LEU:HB3	1:A:728:GLU:HG2	1.80	0.63
1:B:739:ARG:HG3	5:B:348:HOH:O	1.98	0.63
1:B:751:TYR:CZ	1:B:755:ARG:HG3	2.34	0.63
1:B:810:GLU:OE1	1:B:925:ARG:HD2	1.99	0.63
1:D:730:GLY:HA3	1:D:823:TYR:CE1	2.34	0.63
1:C:912:VAL:HG23	1:C:913:ASN:OD1	1.99	0.63
1:A:700:MET:HE1	1:A:746:LEU:HD11	1.81	0.63
1:A:959:PHE:HB3	1:A:977:MET:HG2	1.80	0.62
1:B:979:ARG:HH11	3:B:451:HG9:H602	1.64	0.62
1:C:994:HIS:C	1:C:995:ILE:HD13	2.19	0.62
1:D:763:ILE:H	1:D:805:ASN:HD21	1.46	0.62
1:C:700:MET:HE2	1:C:746:LEU:HD21	1.82	0.62
1:C:751:TYR:CZ	1:C:755:ARG:HG3	2.34	0.62
1:D:881:ARG:O	1:D:885:LEU:HD13	2.00	0.62
4:B:462:666:H28	4:B:462:666:H162	1.82	0.62
1:C:758:PRO:HD3	1:C:1011:GLY:H	1.64	0.61
1:D:1008:LEU:HD23	1:D:1008:LEU:N	2.14	0.61
1:C:719:GLN:HA	1:C:722:ASN:HD22	1.66	0.61
1:C:784:ILE:HG21	1:C:807:PRO:HB3	1.82	0.60
1:D:718:GLN:NE2	1:D:722:ASN:HD21	1.99	0.60
1:D:865:ARG:HG2	1:D:865:ARG:NH1	2.17	0.60
1:C:1013:TRP:CZ3	1:C:1055:ARG:HB3	2.37	0.60
1:B:681:ILE:O	1:B:685:VAL:HG23	2.02	0.60
1:C:703:LEU:HD22	1:C:750:TRP:CE2	2.37	0.60
1:D:829:THR:HG22	4:D:464:666:H182	1.84	0.59
1:C:814:LEU:HD13	1:C:929:CYS:HB3	1.84	0.59
1:B:1069:HIS:HE2	1:B:1073:LYS:HD2	1.67	0.59
1:A:664:VAL:HG12	1:A:668:ASP:OD2	2.01	0.59
1:A:694:ARG:O	1:A:698:GLN:HG2	2.01	0.59
1:B:828:ARG:HG2	1:B:832:PHE:CG	2.38	0.59
1:A:845:ASN:HB3	1:B:887:ILE:HD13	1.84	0.59
1:D:707:THR:HB	1:D:787:ILE:HG21	1.85	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:664:VAL:HG12	1:B:668:ASP:OD2	2.03	0.58
1:C:752:LEU:HD11	1:C:935:LEU:HD22	1.84	0.58
1:D:914:SER:O	1:D:915:ASN:HB2	2.03	0.58
1:B:1014:LEU:O	1:B:1015:GLU:HG2	2.02	0.58
1:B:939:ASN:HD22	1:B:940:GLY:N	2.02	0.58
1:B:730:GLY:HA3	1:B:823:TYR:CE1	2.39	0.58
1:D:716:PRO:CG	1:D:719:GLN:NE2	2.67	0.58
1:B:917:ILE:HG23	1:B:924:ASP:HB3	1.85	0.58
1:B:930:GLN:O	1:B:934:LYS:HG3	2.03	0.58
1:D:719:GLN:NE2	1:D:719:GLN:H	2.01	0.58
1:A:757:VAL:HG13	1:A:1009:LEU:O	2.04	0.58
1:B:700:MET:HE2	1:B:700:MET:HA	1.86	0.57
1:B:698:GLN:NE2	5:B:374:HOH:O	2.37	0.57
1:D:905:PHE:CD1	1:D:931:VAL:HG21	2.39	0.57
1:D:763:ILE:H	1:D:805:ASN:ND2	2.02	0.57
1:B:1003:TYR:HD2	1:B:1009:LEU:HG	1.70	0.57
1:A:730:GLY:HA3	1:A:823:TYR:HE1	1.69	0.57
1:C:700:MET:HE2	1:C:746:LEU:CD2	2.33	0.57
1:D:810:GLU:OE1	1:D:925:ARG:HD2	2.05	0.57
1:A:883:ARG:NH1	1:A:883:ARG:HG2	2.19	0.56
1:C:660:ASP:O	1:C:663:LEU:HB2	2.05	0.56
1:A:995:ILE:N	1:A:995:ILE:HD12	2.20	0.56
1:D:696:LEU:HB3	1:D:728:GLU:HG2	1.87	0.56
1:D:741:HIS:O	1:D:745:VAL:HG23	2.05	0.56
1:D:812:MET:O	1:D:816:VAL:HG23	2.05	0.56
1:A:684:LEU:O	1:A:688:MET:HG3	2.05	0.56
1:D:701:TYR:CZ	1:D:705:GLN:HG3	2.41	0.56
1:C:724:PHE:O	1:C:728:GLU:HG3	2.06	0.56
1:A:804:SER:C	1:A:805:ASN:HD22	2.09	0.56
1:B:874:LEU:HD22	1:B:878:GLU:HB3	1.87	0.55
1:A:881:ARG:HG3	1:A:881:ARG:HH11	1.71	0.55
1:D:763:ILE:O	1:D:765:ASN:N	2.39	0.55
1:A:783:ARG:HG2	1:A:784:ILE:N	2.21	0.55
1:C:1015:GLU:O	1:C:1055:ARG:HD3	2.07	0.55
1:A:979:ARG:NH1	3:A:453:HG9:H602	2.22	0.55
1:D:962:GLN:O	1:D:966:GLU:HG3	2.07	0.55
1:A:912:VAL:O	1:A:913:ASN:HB2	2.07	0.55
1:D:896:LYS:HD3	5:D:373:HOH:O	2.07	0.55
1:D:712:ILE:HD12	1:D:787:ILE:CD1	2.37	0.54
1:C:912:VAL:HG23	1:C:913:ASN:H	1.70	0.54
1:C:1061:LEU:C	1:C:1061:LEU:HD12	2.28	0.54
1:A:751:TYR:CZ	1:A:755:ARG:HG3	2.42	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:734:ILE:HB	1:D:735:PRO:HD2	1.88	0.54
1:D:912:VAL:O	1:D:914:SER:N	2.40	0.54
1:D:716:PRO:CB	1:D:719:GLN:NE2	2.71	0.54
1:A:962:GLN:O	1:A:966:GLU:HG3	2.08	0.54
1:A:828:ARG:HG2	1:A:832:PHE:CG	2.42	0.54
4:A:461:666:H162	4:A:461:666:H28	1.89	0.54
1:B:816:VAL:O	1:B:820:MET:HG3	2.08	0.54
1:D:724:PHE:O	1:D:728:GLU:HG3	2.07	0.54
1:D:787:ILE:HG22	1:D:788:SER:N	2.21	0.54
1:A:708:GLY:HA2	5:A:128:HOH:O	2.07	0.54
1:D:914:SER:O	1:D:915:ASN:CB	2.56	0.54
1:D:714:LYS:HE2	1:D:714:LYS:HA	1.89	0.54
1:D:716:PRO:HG2	1:D:719:GLN:HE21	1.74	0.53
1:A:783:ARG:HG2	1:A:784:ILE:H	1.72	0.53
1:C:1004:ASP:HB2	1:C:1009:LEU:HD12	1.89	0.53
1:B:956:VAL:HG11	1:B:984:LEU:HD13	1.88	0.53
1:D:1061:LEU:HD12	1:D:1062:MET:N	2.23	0.53
1:D:674:MET:CE	1:D:703:LEU:HD21	2.38	0.53
1:B:1009:LEU:HD22	1:B:1061:LEU:CD2	2.36	0.53
1:B:918:GLU:O	1:B:920:SER:N	2.42	0.53
1:C:847:ARG:CZ	1:D:891:LEU:HD13	2.38	0.53
1:D:1069:HIS:NE2	1:D:1073:LYS:HD3	2.23	0.53
1:A:952:THR:O	1:A:956:VAL:HG13	2.08	0.53
1:A:762:GLN:HE22	1:A:801:CYS:H	1.55	0.53
1:D:682:PHE:CE1	1:D:950:LYS:HG2	2.44	0.53
1:A:700:MET:CE	1:A:700:MET:HA	2.39	0.53
1:D:938:ILE:HD12	1:D:996:VAL:HG22	1.91	0.53
1:B:729:ASN:HA	1:B:739:ARG:NH2	2.23	0.53
1:C:905:PHE:CD1	1:C:931:VAL:HG21	2.43	0.53
1:B:1004:ASP:O	1:B:1007:GLY:N	2.40	0.52
1:C:935:LEU:C	1:C:935:LEU:HD23	2.30	0.52
1:D:944:VAL:HG12	1:D:947:LEU:HD12	1.92	0.52
1:B:905:PHE:HA	1:B:927:LEU:CD2	2.38	0.52
1:D:694:ARG:HA	1:D:728:GLU:OE1	2.08	0.52
1:A:1004:ASP:HB2	1:A:1009:LEU:HD12	1.92	0.52
1:C:663:LEU:HD12	1:C:666:GLU:HB2	1.91	0.52
1:B:926:LEU:O	1:B:930:GLN:HG3	2.09	0.52
1:A:817:ALA:O	1:A:821:HIS:HB3	2.10	0.52
1:C:719:GLN:H	1:C:719:GLN:NE2	2.08	0.52
1:B:979:ARG:NH1	3:B:451:HG9:H602	2.25	0.51
1:C:735:PRO:HG2	1:C:958:GLU:HB2	1.91	0.51
1:A:829:THR:HG22	4:A:461:666:H182	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1061:LEU:C	1:D:1061:LEU:HD12	2.31	0.51
1:A:751:TYR:CE2	1:A:755:ARG:HG3	2.46	0.51
1:C:716:PRO:HB2	1:C:719:GLN:NE2	2.26	0.51
1:A:865:ARG:NH2	1:C:874:LEU:O	2.44	0.51
1:C:784:ILE:CG2	1:C:807:PRO:HB3	2.40	0.51
1:D:986:LYS:O	1:D:990:SER:HB2	2.11	0.50
1:B:696:LEU:HB3	1:B:728:GLU:HG2	1.93	0.50
1:D:663:LEU:O	1:D:666:GLU:HB2	2.11	0.50
1:B:700:MET:HE2	1:B:746:LEU:HD21	1.94	0.50
1:B:751:TYR:CE2	1:B:755:ARG:HG3	2.47	0.50
1:A:912:VAL:O	1:A:913:ASN:CB	2.60	0.50
1:C:659:LEU:N	1:C:694:ARG:HH22	2.09	0.50
1:C:679:PHE:HZ	1:C:684:LEU:HD22	1.76	0.50
1:D:784:ILE:HG13	1:D:786:TYR:CE1	2.46	0.50
1:B:817:ALA:O	1:B:821:HIS:HB3	2.11	0.50
1:A:669:SER:O	1:A:673:LYS:HG3	2.12	0.50
1:D:707:THR:HB	1:D:787:ILE:CG2	2.42	0.50
1:D:914:SER:O	1:D:915:ASN:ND2	2.43	0.50
1:D:677:TRP:NE1	1:D:1061:LEU:HB3	2.27	0.50
1:D:700:MET:CE	1:D:746:LEU:CD2	2.90	0.50
1:D:763:ILE:C	1:D:765:ASN:N	2.65	0.49
1:D:1069:HIS:HE2	1:D:1073:LYS:HD3	1.76	0.49
1:A:942:ALA:HB1	1:A:1061:LEU:HB2	1.93	0.49
1:A:881:ARG:O	1:A:885:LEU:HG	2.11	0.49
1:D:844:TYR:CE2	1:D:852:ASN:HB3	2.47	0.49
1:B:666:GLU:O	1:B:669:SER:HB3	2.12	0.49
1:A:705:GLN:OE1	1:A:710:LEU:HD12	2.12	0.49
1:D:866:PRO:HG2	1:D:867:GLU:OE1	2.13	0.49
1:D:787:ILE:CG2	1:D:788:SER:N	2.76	0.49
1:C:969:LEU:HB2	1:C:971:LEU:HD12	1.95	0.49
1:A:810:GLU:OE1	1:A:925:ARG:HD2	2.13	0.49
1:D:753:THR:HG1	1:D:815:TYR:HH	1.56	0.49
1:B:962:GLN:O	1:B:966:GLU:HG3	2.13	0.49
1:C:966:GLU:O	1:C:971:LEU:HB2	2.13	0.49
1:D:913:ASN:O	1:D:915:ASN:N	2.46	0.48
1:C:679:PHE:O	1:C:681:ILE:N	2.44	0.48
1:C:956:VAL:HG11	1:C:984:LEU:HD13	1.95	0.48
1:B:694:ARG:HA	1:B:728:GLU:OE1	2.13	0.48
1:B:897:LYS:NZ	5:B:363:HOH:O	2.46	0.48
1:B:849:VAL:HG23	5:B:100:HOH:O	2.13	0.48
1:D:815:TYR:CD2	1:D:815:TYR:N	2.80	0.48
1:D:955:ILE:HG23	1:D:956:VAL:N	2.27	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:912:VAL:C	1:D:914:SER:N	2.67	0.48
1:D:816:VAL:HG21	1:D:882:PHE:HZ	1.78	0.48
1:D:894:ASP:OD1	1:D:896:LYS:HB3	2.14	0.48
1:A:872:LEU:HD13	1:A:873:HIS:N	2.29	0.48
1:D:901:PHE:O	1:D:904:GLU:HB2	2.14	0.48
1:D:679:PHE:HZ	1:D:684:LEU:CD2	2.20	0.48
1:C:912:VAL:CG2	1:C:913:ASN:N	2.75	0.48
1:D:881:ARG:CG	1:D:881:ARG:HH11	2.24	0.47
1:B:669:SER:O	1:B:672:GLU:HB3	2.14	0.47
1:A:891:LEU:HD13	1:B:847:ARG:CZ	2.44	0.47
1:D:855:ALA:HB2	1:D:890:ILE:HG21	1.95	0.47
1:A:700:MET:CE	1:A:746:LEU:HD11	2.44	0.47
1:C:919:TRP:O	1:C:925:ARG:HD3	2.14	0.47
1:B:700:MET:CE	1:B:746:LEU:CD1	2.91	0.47
1:D:712:ILE:CD1	1:D:787:ILE:HD13	2.45	0.47
1:D:917:ILE:HD12	1:D:924:ASP:HB3	1.96	0.47
1:D:1004:ASP:CB	1:D:1009:LEU:HD12	2.44	0.47
1:C:711:GLU:OE1	1:C:714:LYS:NZ	2.42	0.47
1:D:1009:LEU:HD23	1:D:1010:PRO:HD2	1.97	0.47
1:C:846:ASP:OD2	1:D:883:ARG:NH1	2.45	0.47
1:A:924:ASP:O	1:A:928:VAL:HG23	2.14	0.47
1:B:865:ARG:HD3	1:B:867:GLU:OE2	2.15	0.47
1:B:945:ARG:O	1:B:949:LEU:HG	2.15	0.47
1:D:1014:LEU:O	1:D:1015:GLU:O	2.32	0.47
1:B:993:THR:OG1	1:B:1069:HIS:HE1	1.97	0.47
1:C:718:GLN:HG3	1:C:722:ASN:HD21	1.79	0.47
1:A:805:ASN:N	1:A:805:ASN:HD22	2.11	0.47
1:B:912:VAL:HG12	1:B:913:ASN:ND2	2.30	0.47
1:D:760:LEU:HD23	1:D:800:GLY:O	2.15	0.47
1:D:762:GLN:OE1	1:D:804:SER:CB	2.62	0.47
1:B:917:ILE:HG22	1:B:918:GLU:N	2.29	0.46
1:C:1004:ASP:CB	1:C:1009:LEU:HD12	2.45	0.46
1:B:938:ILE:HD11	1:B:999:LEU:HD23	1.96	0.46
1:B:994:HIS:HB2	1:B:995:ILE:HD12	1.97	0.46
1:A:902:LEU:HD11	1:A:1002:SER:OG	2.15	0.46
1:A:703:LEU:HD22	1:A:750:TRP:CE2	2.50	0.46
1:C:912:VAL:CG2	1:C:913:ASN:H	2.29	0.46
1:A:814:LEU:HD11	1:A:933:ILE:HB	1.97	0.46
1:D:1007:GLY:C	1:D:1008:LEU:HD23	2.35	0.46
1:B:816:VAL:O	1:B:819:ALA:HB3	2.15	0.46
1:D:716:PRO:HG2	1:D:719:GLN:NE2	2.31	0.46
1:A:823:TYR:HE2	1:A:857:SER:HB3	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:694:ARG:HD2	1:D:725:ARG:HG2	1.97	0.46
1:D:700:MET:CE	1:D:746:LEU:HD21	2.45	0.46
1:C:845:ASN:HB3	1:D:887:ILE:HD13	1.98	0.46
1:B:939:ASN:ND2	1:B:940:GLY:N	2.63	0.46
1:D:1013:TRP:HA	1:D:1057:ILE:CG2	2.44	0.46
1:D:960:TYR:HB3	1:D:979:ARG:CZ	2.45	0.46
1:D:734:ILE:HD11	1:D:737:HIS:HB2	1.98	0.45
1:C:695:ILE:O	1:C:699:VAL:HG23	2.15	0.45
1:B:918:GLU:C	1:B:920:SER:H	2.20	0.45
1:B:762:GLN:OE1	1:B:762:GLN:HA	2.16	0.45
1:D:715:ILE:HG23	1:D:870:PHE:HB2	1.97	0.45
1:D:845:ASN:O	1:D:847:ARG:HG3	2.15	0.45
1:D:691:LYS:HE2	1:D:691:LYS:HB3	1.83	0.45
1:C:703:LEU:HD22	1:C:750:TRP:CD2	2.51	0.45
1:D:670:LEU:HD23	1:D:670:LEU:O	2.16	0.45
1:D:859:TRP:CZ2	1:D:883:ARG:HA	2.51	0.45
1:A:859:TRP:CE2	1:A:883:ARG:HD2	2.51	0.45
1:C:732:ARG:HH11	1:C:826:PRO:HA	1.80	0.45
1:D:794:ASN:OD1	1:D:800:GLY:HA2	2.16	0.45
1:B:1014:LEU:H	1:B:1014:LEU:CD1	2.17	0.45
1:B:783:ARG:HH11	1:B:783:ARG:HG2	1.82	0.45
1:A:960:TYR:HB3	1:A:979:ARG:CZ	2.47	0.45
1:A:851:GLU:HB3	1:A:891:LEU:HD23	1.99	0.45
1:C:762:GLN:HA	1:C:805:ASN:HD21	1.82	0.45
1:C:729:ASN:HA	1:C:739:ARG:HH22	1.81	0.45
1:A:944:VAL:HG12	1:A:947:LEU:HD22	1.99	0.45
1:C:1061:LEU:HD12	1:C:1062:MET:N	2.32	0.45
1:B:700:MET:HE2	1:B:746:LEU:CD2	2.46	0.44
1:D:737:HIS:NE2	5:D:45:HOH:O	2.36	0.44
1:D:847:ARG:O	1:D:848:SER:C	2.54	0.44
1:C:851:GLU:OE1	1:C:894:ASP:HB2	2.17	0.44
1:C:832:PHE:O	1:C:835:ALA:N	2.50	0.44
1:B:804:SER:C	1:B:805:ASN:HD22	2.20	0.44
1:A:869:ASN:ND2	1:A:872:LEU:HB3	2.33	0.44
1:A:758:PRO:HG3	1:A:799:TYR:CE2	2.51	0.44
1:B:909:ALA:HB2	1:B:917:ILE:CD1	2.41	0.44
1:D:944:VAL:O	1:D:945:ARG:C	2.56	0.44
1:D:871:LEU:O	1:D:874:LEU:HB2	2.18	0.44
1:D:738:ASN:HB2	5:D:342:HOH:O	2.18	0.44
1:C:847:ARG:O	1:C:848:SER:C	2.55	0.44
1:B:670:LEU:HA	1:B:673:LYS:NZ	2.32	0.44
1:C:718:GLN:O	1:C:722:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:674:MET:HE1	1:D:703:LEU:HD21	2.00	0.44
1:C:739:ARG:HG3	5:C:311:HOH:O	2.18	0.44
1:A:872:LEU:N	1:A:872:LEU:HD12	2.33	0.43
1:A:891:LEU:HD13	1:B:847:ARG:NH1	2.33	0.43
1:A:881:ARG:HG3	1:A:881:ARG:NH1	2.31	0.43
1:C:846:ASP:CG	1:D:883:ARG:HH12	2.21	0.43
1:D:712:ILE:HD12	1:D:787:ILE:HD11	2.00	0.43
1:C:915:ASN:O	1:C:916:GLY:O	2.37	0.43
1:B:696:LEU:N	1:B:728:GLU:OE2	2.51	0.43
1:C:748:ALA:HB2	5:C:337:HOH:O	2.18	0.43
1:C:670:LEU:CD2	1:C:674:MET:SD	3.07	0.43
1:B:670:LEU:O	1:B:674:MET:HG3	2.17	0.43
1:B:674:MET:C	1:B:676:ASN:H	2.21	0.43
1:B:758:PRO:HB2	1:B:1057:ILE:HD13	1.99	0.43
1:D:757:VAL:HG13	1:D:1009:LEU:O	2.18	0.43
1:B:694:ARG:O	1:B:698:GLN:HG2	2.19	0.43
1:C:1060:GLN:O	1:C:1063:HIS:HB3	2.18	0.43
1:A:796:ASP:OD1	1:A:798:SER:OG	2.12	0.43
1:D:1009:LEU:HA	1:D:1010:PRO:HD2	1.91	0.43
1:D:663:LEU:HA	1:D:666:GLU:OE1	2.19	0.43
1:A:758:PRO:HG3	1:A:799:TYR:HE2	1.84	0.43
1:C:670:LEU:HD23	1:C:674:MET:SD	2.59	0.43
1:D:1055:ARG:CG	1:D:1056:ARG:H	2.32	0.43
1:B:729:ASN:HA	1:B:739:ARG:HH22	1.82	0.43
1:B:674:MET:CE	1:B:699:VAL:HG13	2.48	0.43
1:D:952:THR:O	1:D:956:VAL:HG13	2.19	0.43
1:B:810:GLU:HG2	1:B:885:LEU:HD13	2.01	0.43
1:B:812:MET:HG2	1:B:882:PHE:HE1	1.83	0.43
1:D:700:MET:HE3	1:D:746:LEU:CD2	2.49	0.42
1:A:994:HIS:HB2	1:A:995:ILE:HD12	2.00	0.42
1:B:908:LYS:HD2	1:B:924:ASP:OD1	2.19	0.42
1:D:750:TRP:CZ2	1:D:755:ARG:NH2	2.85	0.42
1:B:758:PRO:HB3	1:B:1013:TRP:CE2	2.55	0.42
1:B:918:GLU:C	1:B:920:SER:N	2.72	0.42
1:C:743:THR:O	1:C:746:LEU:HB3	2.20	0.42
1:C:807:PRO:HG2	1:C:810:GLU:CD	2.40	0.42
1:D:852:ASN:OD1	1:D:891:LEU:HD21	2.18	0.42
1:A:811:LEU:HA	1:A:811:LEU:HD23	1.86	0.42
1:D:712:ILE:HD12	1:D:787:ILE:HD13	2.00	0.42
1:D:755:ARG:O	1:D:757:VAL:HG23	2.19	0.42
1:D:874:LEU:HG	1:D:878:GLU:OE2	2.19	0.42
1:A:679:PHE:HD1	1:A:680:PRO:HD2	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1055:ARG:CG	1:D:1056:ARG:N	2.82	0.42
1:B:941:PRO:HD3	4:B:462:666:C40	2.50	0.42
1:A:669:SER:O	1:A:672:GLU:HB3	2.19	0.42
1:C:755:ARG:NH2	1:C:789:SER:OG	2.52	0.42
1:C:763:ILE:CG1	1:C:764:HIS:N	2.80	0.42
1:D:1062:MET:HE2	1:D:1062:MET:HA	2.01	0.42
4:D:464:666:H181	5:D:320:HOH:O	2.20	0.42
1:D:990:SER:HB3	4:D:464:666:I54	2.90	0.42
1:B:714:LYS:HE3	1:B:714:LYS:HA	2.02	0.42
1:A:983:GLN:OE1	1:A:986:LYS:HD3	2.20	0.42
1:B:865:ARG:HG3	1:B:865:ARG:HH11	1.84	0.42
1:D:806:ILE:HA	1:D:807:PRO:HD2	1.93	0.41
1:A:758:PRO:HB3	1:A:1013:TRP:CE2	2.55	0.41
1:D:935:LEU:HD12	1:D:935:LEU:HA	1.92	0.41
1:B:691:LYS:HE3	1:B:694:ARG:HH21	1.85	0.41
1:D:1062:MET:HB2	1:D:1062:MET:HE3	1.92	0.41
1:A:956:VAL:HG11	1:A:984:LEU:HD13	2.01	0.41
1:C:681:ILE:O	1:C:685:VAL:HG23	2.20	0.41
1:B:812:MET:HG2	1:B:882:PHE:CE1	2.55	0.41
1:D:691:LYS:HE3	1:D:694:ARG:NH2	2.35	0.41
1:D:695:ILE:HG23	1:D:696:LEU:N	2.35	0.41
1:C:700:MET:HE3	1:C:746:LEU:HD13	2.00	0.41
1:D:939:ASN:HD22	1:D:943:LYS:HG2	1.86	0.41
1:B:959:PHE:HB3	1:B:977:MET:HG2	2.00	0.41
1:A:847:ARG:HB3	5:A:229:HOH:O	2.20	0.41
1:B:807:PRO:HD2	1:B:925:ARG:HD3	2.02	0.41
1:C:939:ASN:ND2	1:C:939:ASN:C	2.73	0.41
1:D:860:ASN:C	1:D:860:ASN:ND2	2.74	0.41
1:B:1014:LEU:O	1:B:1015:GLU:CB	2.68	0.41
1:D:700:MET:HE3	1:D:746:LEU:HD22	2.02	0.41
1:D:1013:TRP:CZ3	1:D:1055:ARG:HB3	2.56	0.41
1:D:713:PHE:O	1:D:714:LYS:C	2.58	0.41
1:B:1007:GLY:HA2	5:B:251:HOH:O	2.21	0.41
1:B:821:HIS:NE2	1:B:822:ASP:OD2	2.53	0.41
1:C:952:THR:O	1:C:956:VAL:HG13	2.20	0.41
1:B:760:LEU:HD23	1:B:801:CYS:N	2.35	0.41
1:A:677:TRP:O	1:A:943:LYS:HE2	2.20	0.41
1:A:671:ILE:HA	1:A:671:ILE:HD13	1.93	0.41
1:B:952:THR:HG23	1:B:988:GLN:NE2	2.35	0.41
1:C:674:MET:HE3	1:C:699:VAL:HG13	2.03	0.41
1:A:845:ASN:O	1:A:846:ASP:HB2	2.21	0.41
1:B:953:GLU:O	1:B:956:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:872:LEU:N	1:D:872:LEU:HD12	2.35	0.41
1:C:887:ILE:HD13	1:D:845:ASN:HB3	2.03	0.41
1:A:741:HIS:O	1:A:745:VAL:HG23	2.21	0.41
1:D:881:ARG:NH1	1:D:881:ARG:HG3	2.32	0.41
1:B:783:ARG:NH1	1:B:783:ARG:HG2	2.36	0.41
1:C:663:LEU:HD13	1:C:666:GLU:OE1	2.20	0.40
1:D:942:ALA:HB1	1:D:1061:LEU:HB2	2.03	0.40
1:C:847:ARG:O	1:C:849:VAL:N	2.54	0.40
1:D:683:GLU:O	1:D:686:GLU:HB3	2.20	0.40
1:C:998:PRO:HA	5:C:424:HOH:O	2.21	0.40
1:C:909:ALA:HB2	1:C:917:ILE:CD1	2.52	0.40
1:A:1061:LEU:N	1:A:1061:LEU:HD23	2.20	0.40
1:B:755:ARG:HD2	5:B:387:HOH:O	2.20	0.40
1:D:904:GLU:O	1:D:905:PHE:C	2.60	0.40
1:C:1057:ILE:HD12	1:C:1057:ILE:O	2.21	0.40
1:D:688:MET:HE2	1:D:691:LYS:O	2.21	0.40
1:C:960:TYR:HB3	1:C:979:ARG:CZ	2.52	0.40
1:B:748:ALA:HB3	1:B:936:ALA:HB1	2.04	0.40
1:B:897:LYS:HB3	1:B:897:LYS:HE2	1.91	0.40
1:A:674:MET:C	1:A:676:ASN:H	2.25	0.40
1:D:780:ASN:HD22	1:D:780:ASN:N	2.20	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	357/420 (85%)	337 (94%)	18 (5%)	2 (1%)	33	47
1	B	357/420 (85%)	325 (91%)	26 (7%)	6 (2%)	14	17
1	C	366/420 (87%)	336 (92%)	25 (7%)	5 (1%)	16	22
1	D	359/420 (86%)	319 (89%)	31 (9%)	9 (2%)	9	8
All	All	1439/1680 (86%)	1317 (92%)	100 (7%)	22 (2%)	15	20

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	912	VAL
1	B	913	ASN
1	C	660	ASP
1	D	914	SER
1	D	1015	GLU
1	A	869	ASN
1	B	919	TRP
1	C	848	SER
1	C	916	GLY
1	D	764	HIS
1	A	660	ASP
1	B	689	GLY
1	D	848	SER
1	D	908	LYS
1	D	909	ALA
1	C	912	VAL
1	D	796	ASP
1	D	915	ASN
1	C	662	ILE
1	B	763	ILE
1	D	758	PRO
1	B	940	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	310/370 (84%)	293 (94%)	17 (6%)	30	46
1	B	308/370 (83%)	295 (96%)	13 (4%)	40	60
1	C	313/370 (85%)	301 (96%)	12 (4%)	44	65
1	D	308/370 (83%)	288 (94%)	20 (6%)	24	36
All	All	1239/1480 (84%)	1177 (95%)	62 (5%)	34	51

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	666	GLU
1	A	694	ARG
1	A	700	MET
1	A	706	ASP
1	A	792	CYS
1	A	820	MET
1	A	828	ARG
1	A	872	LEU
1	A	883	ARG
1	A	915	ASN
1	A	918	GLU
1	A	939	ASN
1	A	947	LEU
1	A	965	GLU
1	A	1056	ARG
1	A	1061	LEU
1	A	1069	HIS
1	B	665	GLU
1	B	705	GLN
1	B	714	LYS
1	B	719	GLN
1	B	755	ARG
1	B	820	MET
1	B	828	ARG
1	B	872	LEU
1	B	939	ASN
1	B	946	ASP
1	B	947	LEU
1	B	1014	LEU
1	B	1015	GLU
1	C	669	SER
1	C	705	GLN
1	C	711	GLU
1	C	719	GLN
1	C	780	ASN
1	C	792	CYS
1	C	820	MET
1	C	828	ARG
1	C	869	ASN
1	C	939	ASN
1	C	947	LEU
1	C	1061	LEU
1	D	670	LEU

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Mol	Chain	Res	Type
1	D	705	GLN
1	D	719	GLN
1	D	781	HIS
1	D	788	SER
1	D	796	ASP
1	D	821	HIS
1	D	847	ARG
1	D	857	SER
1	D	860	ASN
1	D	872	LEU
1	D	875	ASP
1	D	910	ASN
1	D	911	ASP
1	D	917	ILE
1	D	939	ASN
1	D	946	ASP
1	D	990	SER
1	D	1008	LEU
1	D	1057	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	762	GLN
1	A	764	HIS
1	A	805	ASN
1	A	923	ASN
1	A	939	ASN
1	A	1012	GLN
1	B	698	GLN
1	B	705	GLN
1	B	718	GLN
1	B	719	GLN
1	B	722	ASN
1	B	805	ASN
1	B	869	ASN
1	B	923	ASN
1	B	939	ASN
1	B	994	HIS
1	B	1060	GLN
1	B	1069	HIS
1	C	705	GLN

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Mol	Chain	Res	Type
1	C	718	GLN
1	C	719	GLN
1	C	722	ASN
1	C	805	ASN
1	C	869	ASN
1	C	923	ASN
1	C	939	ASN
1	D	718	GLN
1	D	719	GLN
1	D	729	ASN
1	D	805	ASN
1	D	860	ASN
1	D	876	HIS
1	D	898	HIS
1	D	913	ASN
1	D	923	ASN
1	D	939	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 for Mogul analysis.

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HG9	A	453	-	23,23,24	1.43	4 (17%)	28,28,29	2.69	3 (10%)
3	HG9	A	454	-	23,23,24	1.77	5 (21%)	28,28,29	2.71	5 (17%)
4	666	A	461	-	33,33,33	3.61	26 (78%)	46,46,46	2.57	13 (28%)
3	HG9	B	451	-	23,23,24	2.02	6 (26%)	28,28,29	2.74	4 (14%)
3	HG9	B	452	-	23,23,24	1.80	4 (17%)	28,28,29	2.76	6 (21%)
4	666	B	462	-	33,33,33	3.55	24 (72%)	46,46,46	2.56	11 (23%)
4	666	C	463	-	33,33,33	3.61	25 (75%)	46,46,46	2.63	11 (23%)
4	666	D	464	-	33,33,33	3.65	25 (75%)	46,46,46	2.68	15 (32%)

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	HG9	A	453	-	-	0/32/32/33	0/0/0/0
3	HG9	A	454	-	-	0/32/32/33	0/0/0/0
4	666	A	461	-	-	0/12/39/39	0/4/4/4
3	HG9	B	451	-	-	0/32/32/33	0/0/0/0
3	HG9	B	452	-	-	0/32/32/33	0/0/0/0
4	666	B	462	-	-	0/12/39/39	0/4/4/4
4	666	C	463	-	-	0/12/39/39	0/4/4/4
4	666	D	464	-	-	0/12/39/39	0/4/4/4

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	464	666	C15-N26	8.92	1.49	1.34
4	A	461	666	C15-N26	8.79	1.49	1.34
4	B	462	666	C15-N26	8.50	1.49	1.34
4	C	463	666	C15-N26	8.19	1.48	1.34
4	B	462	666	C37-N38	8.02	1.39	1.29
4	A	461	666	C37-N38	7.79	1.38	1.29
4	D	464	666	C37-N38	7.35	1.38	1.29
4	C	463	666	C37-N38	6.46	1.37	1.29
4	C	463	666	C4-C5	6.28	1.49	1.38
4	B	462	666	C17-C18	6.15	1.72	1.51
4	D	464	666	C4-C5	6.08	1.49	1.38
3	B	452	HG9	C9-C12	-5.90	1.52	1.55
4	D	464	666	C17-C18	5.83	1.71	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	461	666	C17-C18	5.72	1.71	1.51
4	A	461	666	C4-C5	5.65	1.48	1.38
4	D	464	666	C16-C15	5.64	1.57	1.49
4	C	463	666	C17-C18	5.61	1.70	1.51
4	B	462	666	C4-C5	5.34	1.48	1.38
4	C	463	666	C19-C12	5.16	1.58	1.46
3	B	451	HG9	C9-C12	-5.11	1.53	1.55
4	A	461	666	C19-C12	5.06	1.58	1.46
4	B	462	666	C19-C12	5.05	1.58	1.46
4	A	461	666	C16-C15	4.91	1.56	1.49
4	B	462	666	C16-C15	4.64	1.55	1.49
4	C	463	666	C4-C3	4.64	1.47	1.39
4	C	463	666	C16-C15	4.59	1.55	1.49
4	D	464	666	C42-C37	4.46	1.58	1.50
4	A	461	666	C42-C37	4.32	1.58	1.50
4	D	464	666	C19-C12	4.21	1.56	1.46
4	B	462	666	C2-C3	4.07	1.48	1.38
4	C	463	666	C11-C3	4.02	1.58	1.51
3	A	454	HG9	C27-C30	4.02	1.61	1.51
4	C	463	666	C42-C37	4.01	1.57	1.50
3	B	452	HG9	C27-C30	4.00	1.61	1.51
4	B	462	666	C42-C37	3.95	1.57	1.50
4	A	461	666	N39-N38	-3.95	1.27	1.38
3	B	451	HG9	C36-C37	3.87	1.58	1.52
4	D	464	666	C32-C27	3.78	1.45	1.39
4	D	464	666	C4-C3	3.72	1.46	1.39
3	A	453	HG9	C27-C30	3.70	1.60	1.51
3	A	454	HG9	C9-C12	-3.69	1.53	1.55
4	A	461	666	C4-C3	3.61	1.45	1.39
4	C	463	666	N39-N38	-3.57	1.28	1.38
4	D	464	666	C31-C30	3.53	1.45	1.39
4	D	464	666	C2-C3	3.51	1.46	1.38
4	C	463	666	C27-N26	-3.46	1.35	1.41
4	C	463	666	C2-C3	3.45	1.46	1.38
3	B	451	HG9	C27-C30	3.37	1.59	1.51
4	C	463	666	C11-C12	3.37	1.55	1.51
4	A	461	666	C2-C3	3.36	1.46	1.38
4	D	464	666	C41-C42	3.36	1.57	1.52
4	D	464	666	C41-C40	3.35	1.56	1.50
3	A	454	HG9	C36-N33	3.35	1.53	1.47
3	A	454	HG9	C36-C37	3.35	1.57	1.52
4	D	464	666	N39-N38	-3.32	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	453	HG9	C36-C37	3.28	1.57	1.52
3	B	451	HG9	C36-N33	3.26	1.53	1.47
4	B	462	666	C41-C42	3.25	1.57	1.52
4	B	462	666	N39-N38	-3.24	1.29	1.38
4	B	462	666	C4-C3	3.23	1.45	1.39
3	B	451	HG9	C30-N33	3.22	1.43	1.35
4	A	461	666	C31-C30	3.22	1.44	1.39
4	C	463	666	C31-C30	3.21	1.44	1.39
4	C	463	666	C41-C42	3.20	1.57	1.52
4	A	461	666	C27-N26	-3.18	1.35	1.41
4	C	463	666	C32-C27	3.16	1.44	1.39
4	C	463	666	C41-C40	3.15	1.56	1.50
4	B	462	666	C32-C27	3.10	1.44	1.39
4	A	461	666	C18-C19	3.06	1.55	1.50
4	A	461	666	C1-C6	3.02	1.46	1.39
4	B	462	666	C41-C40	2.99	1.55	1.50
4	C	463	666	C29-C30	2.99	1.44	1.39
4	D	464	666	C11-C3	2.98	1.56	1.51
4	B	462	666	C1-C2	2.97	1.45	1.39
4	A	461	666	C32-C27	2.93	1.44	1.39
4	A	461	666	C32-C31	2.89	1.44	1.38
4	D	464	666	C32-C31	2.89	1.44	1.38
4	B	462	666	C31-C30	2.78	1.44	1.39
4	D	464	666	C29-C30	2.72	1.44	1.39
4	A	461	666	C40-N39	2.71	1.37	1.34
4	B	462	666	C29-C30	2.70	1.44	1.39
4	D	464	666	C18-C19	2.69	1.54	1.50
4	C	463	666	C1-C6	2.69	1.45	1.39
3	B	451	HG9	C37-C40	2.66	1.59	1.53
4	B	462	666	C18-C19	2.66	1.54	1.50
4	D	464	666	C17-C16	2.64	1.60	1.51
4	B	462	666	C1-C6	2.56	1.44	1.39
4	B	462	666	C27-N26	-2.55	1.36	1.41
4	C	463	666	C1-C2	2.54	1.44	1.39
4	A	461	666	C41-C40	2.51	1.54	1.50
4	D	464	666	C27-N26	-2.40	1.37	1.41
4	C	463	666	C28-C27	2.39	1.43	1.39
4	B	462	666	C28-C27	2.39	1.43	1.39
4	A	461	666	C29-C30	2.35	1.43	1.39
4	A	461	666	C17-C16	2.34	1.59	1.51
4	D	464	666	C11-C12	2.32	1.54	1.51
4	C	463	666	C6-C5	2.32	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	462	666	C11-C3	2.31	1.55	1.51
4	B	462	666	C17-C16	2.27	1.59	1.51
4	A	461	666	C6-C5	2.25	1.44	1.38
3	B	452	HG9	C30-N33	2.24	1.40	1.35
4	A	461	666	C11-C12	2.21	1.54	1.51
3	A	453	HG9	C36-N33	2.21	1.51	1.47
4	A	461	666	C28-C27	2.19	1.42	1.39
4	C	463	666	C32-C31	2.18	1.42	1.38
3	B	452	HG9	C36-C37	2.17	1.56	1.52
4	A	461	666	C1-C2	2.16	1.44	1.39
3	A	454	HG9	C37-C40	2.13	1.57	1.53
4	B	462	666	C40-N39	2.13	1.37	1.34
4	C	463	666	C18-C19	2.13	1.53	1.50
4	D	464	666	C1-C2	2.11	1.43	1.39
4	D	464	666	C6-C5	2.11	1.43	1.38
4	A	461	666	C5-I54	2.10	2.16	2.10
4	D	464	666	C28-C27	2.08	1.42	1.39
4	C	463	666	C17-C16	2.08	1.58	1.51
4	D	464	666	C1-C6	2.07	1.43	1.39
4	B	462	666	C32-C31	2.05	1.42	1.38
3	A	453	HG9	C30-N33	2.03	1.40	1.35
4	A	461	666	O46-C40	-2.02	1.18	1.23

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	451	HG9	C37-C36-N33	13.12	132.19	113.35
3	B	452	HG9	C37-C36-N33	12.91	131.88	113.35
3	A	453	HG9	C37-C36-N33	12.55	131.38	113.35
3	A	454	HG9	C37-C36-N33	12.00	130.58	113.35
4	B	462	666	C11-C12-C19	-8.94	102.99	118.13
4	D	464	666	C11-C12-C19	-8.73	103.33	118.13
4	A	461	666	C11-C12-C19	-8.19	104.26	118.13
4	D	464	666	C37-N38-N39	7.96	125.83	117.39
4	C	463	666	C19-C12-C15	-7.76	113.59	120.29
4	C	463	666	C11-C12-C19	-7.46	105.49	118.13
4	C	463	666	C37-N38-N39	7.10	124.92	117.39
4	B	462	666	C37-N38-N39	7.07	124.89	117.39
4	A	461	666	C37-N38-N39	7.00	124.82	117.39
4	A	461	666	C19-C12-C15	-6.89	114.34	120.29
4	B	462	666	C19-C12-C15	-6.22	114.92	120.29
4	D	464	666	C19-C12-C15	-5.88	115.21	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	464	666	C42-C37-N38	-5.77	115.71	123.68
4	B	462	666	C42-C37-N38	-5.41	116.22	123.68
4	C	463	666	C42-C37-N38	-5.26	116.42	123.68
4	A	461	666	C42-C37-N38	-5.02	116.75	123.68
4	D	464	666	C12-C15-N26	-4.79	112.75	122.12
4	C	463	666	C12-C15-N26	-4.77	112.78	122.12
4	A	461	666	C12-C15-N26	-4.73	112.86	122.12
4	B	462	666	C12-C15-N26	-4.53	113.25	122.12
4	C	463	666	C30-C37-N38	4.45	122.10	116.27
3	A	454	HG9	C35-N33-C36	4.39	121.58	116.29
4	D	464	666	C27-N26-C15	4.25	136.44	127.49
4	B	462	666	C30-C37-N38	4.08	121.62	116.27
4	B	462	666	C27-N26-C15	3.95	135.81	127.49
4	A	461	666	C27-N26-C15	3.92	135.73	127.49
4	C	463	666	C27-N26-C15	3.90	135.71	127.49
4	A	461	666	C30-C37-N38	3.65	121.05	116.27
3	A	453	HG9	C60-C35-N33	3.31	121.17	112.30
3	A	454	HG9	C36-C37-C40	3.24	119.08	109.82
4	C	463	666	C6-C5-C4	-3.13	117.53	121.28
4	C	463	666	C16-C15-N26	3.10	123.23	117.90
4	A	461	666	C16-C15-N26	3.08	123.18	117.90
4	D	464	666	C30-C37-N38	3.07	120.30	116.27
3	A	454	HG9	C60-C35-N33	3.04	120.45	112.30
4	D	464	666	C16-C15-N26	2.99	123.04	117.90
4	B	462	666	C16-C15-N26	2.95	122.96	117.90
3	A	453	HG9	C35-N33-C36	2.92	119.81	116.29
4	D	464	666	C3-C11-C12	-2.90	109.03	114.31
4	A	461	666	C6-C5-C4	-2.89	117.83	121.28
3	B	451	HG9	C36-C37-C40	2.88	118.05	109.82
3	B	452	HG9	C35-N33-C36	2.86	119.74	116.29
3	B	452	HG9	O53-C42-C43	-2.69	102.94	109.20
4	D	464	666	C17-C18-C19	2.63	118.14	113.60
4	C	463	666	C18-C17-C16	-2.62	103.22	112.14
4	A	461	666	O46-C40-N39	2.48	123.36	121.06
4	A	461	666	C18-C17-C16	-2.46	103.74	112.14
4	C	463	666	O46-C40-N39	2.46	123.35	121.06
4	B	462	666	C18-C17-C16	-2.45	103.78	112.14
4	D	464	666	C6-C5-C4	-2.41	118.39	121.28
4	A	461	666	C17-C18-C19	2.41	117.77	113.60
4	B	462	666	O46-C40-N39	2.40	123.29	121.06
3	A	454	HG9	C35-N33-C30	-2.39	113.26	120.97
4	D	464	666	O46-C40-N39	2.38	123.27	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	464	666	C30-C37-C42	2.37	123.91	119.44
4	B	462	666	C17-C18-C19	2.29	117.56	113.60
3	B	451	HG9	C60-C35-N33	2.22	118.25	112.30
3	B	452	HG9	O44-C43-C42	-2.17	106.19	111.05
4	D	464	666	C18-C17-C16	-2.14	104.83	112.14
3	B	451	HG9	C35-N33-C36	2.07	118.79	116.29
4	D	464	666	C11-C12-C15	2.06	128.09	123.19
4	A	461	666	C29-C30-C37	-2.04	118.32	120.74
3	B	452	HG9	C60-C35-N33	2.04	117.76	112.30
3	B	452	HG9	C36-C37-C40	2.01	115.58	109.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	363/420 (86%)	0.25	34 (9%) 9 8	26, 42, 69, 77	0
1	B	363/420 (86%)	0.24	30 (8%) 11 10	23, 43, 70, 79	0
1	C	372/420 (88%)	0.37	34 (9%) 9 8	34, 49, 72, 78	0
1	D	365/420 (86%)	0.67	48 (13%) 4 4	33, 55, 74, 79	0
All	All	1463/1680 (87%)	0.38	146 (9%) 8 7	23, 48, 72, 79	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1016	ALA	8.6
1	A	659	LEU	8.1
1	A	662	ILE	7.4
1	C	661	LEU	7.3
1	A	1053	SER	7.2
1	B	662	ILE	6.4
1	B	659	LEU	6.3
1	C	664	VAL	6.3
1	D	659	LEU	6.1
1	D	912	VAL	6.1
1	A	661	LEU	5.7
1	C	662	ILE	5.6
1	D	662	ILE	5.3
1	B	661	LEU	5.3
1	B	660	ASP	5.2
1	A	1055	ARG	5.2
1	A	764	HIS	5.0
1	A	765	ASN	5.0
1	A	766	GLY	5.0
1	D	780	ASN	4.8
1	C	912	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	767	CYS	4.8
1	D	1056	ARG	4.7
1	D	661	LEU	4.6
1	C	764	HIS	4.6
1	A	1054	ARG	4.5
1	D	795	PRO	4.4
1	B	1055	ARG	4.4
1	C	665	GLU	4.3
1	D	784	ILE	4.3
1	D	660	ASP	4.2
1	C	765	ASN	4.2
1	D	1017	GLU	4.1
1	A	660	ASP	4.1
1	D	663	LEU	4.0
1	C	913	ASN	3.9
1	D	665	GLU	3.9
1	D	781	HIS	3.9
1	B	765	ASN	3.8
1	B	1053	SER	3.8
1	B	764	HIS	3.8
1	A	663	LEU	3.7
1	C	766	GLY	3.7
1	C	1053	SER	3.7
1	D	1014	LEU	3.7
1	C	1054	ARG	3.7
1	D	765	ASN	3.6
1	B	663	LEU	3.6
1	C	1015	GLU	3.5
1	C	914	SER	3.5
1	D	815	TYR	3.5
1	D	1055	ARG	3.5
1	C	663	LEU	3.5
1	D	749	VAL	3.5
1	B	912	VAL	3.5
1	A	783	ARG	3.4
1	D	766	GLY	3.4
1	B	766	GLY	3.3
1	D	914	SER	3.3
1	C	779	ILE	3.3
1	A	749	VAL	3.3
1	C	749	VAL	3.3
1	D	819	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	782	GLY	3.2
1	D	764	HIS	3.2
1	C	780	ASN	3.2
1	A	665	GLU	3.2
1	D	748	ALA	3.1
1	C	1055	ARG	3.0
1	C	746	LEU	3.0
1	C	1056	ARG	3.0
1	A	933	ILE	3.0
1	D	664	VAL	3.0
1	A	817	ALA	3.0
1	D	746	LEU	2.9
1	D	936	ALA	2.9
1	D	913	ASN	2.9
1	A	1056	ARG	2.9
1	A	748	ALA	2.9
1	C	748	ALA	2.8
1	A	932	CYS	2.8
1	A	784	ILE	2.8
1	C	659	LEU	2.8
1	B	819	ALA	2.8
1	B	691	LYS	2.8
1	A	818	ALA	2.7
1	D	1015	GLU	2.7
1	B	818	ALA	2.7
1	D	933	ILE	2.7
1	D	798	SER	2.7
1	D	1012	GLN	2.7
1	A	912	VAL	2.7
1	A	664	VAL	2.7
1	D	816	VAL	2.7
1	D	799	TYR	2.7
1	B	816	VAL	2.6
1	D	745	VAL	2.6
1	A	913	ASN	2.6
1	D	935	LEU	2.6
1	D	762	GLN	2.6
1	C	936	ALA	2.6
1	D	711	GLU	2.6
1	B	762	GLN	2.6
1	C	915	ASN	2.6
1	B	913	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	911	ASP	2.5
1	D	915	ASN	2.5
1	D	1057	ILE	2.5
1	D	750	TRP	2.5
1	A	1015	GLU	2.5
1	D	818	ALA	2.5
1	B	746	LEU	2.4
1	A	816	VAL	2.4
1	B	763	ILE	2.4
1	D	814	LEU	2.4
1	B	817	ALA	2.4
1	C	776	ASP	2.4
1	A	745	VAL	2.4
1	B	665	GLU	2.4
1	B	745	VAL	2.3
1	B	664	VAL	2.3
1	B	936	ALA	2.3
1	D	1013	TRP	2.3
1	C	774	ASP	2.2
1	B	1056	ARG	2.2
1	A	815	TYR	2.2
1	A	814	LEU	2.2
1	A	763	ILE	2.2
1	C	911	ASP	2.2
1	D	752	LEU	2.1
1	C	777	GLY	2.1
1	A	746	LEU	2.1
1	B	1014	LEU	2.1
1	D	911	ASP	2.1
1	C	763	ILE	2.1
1	D	787	ILE	2.1
1	A	1057	ILE	2.1
1	B	815	TYR	2.1
1	C	818	ALA	2.0
1	C	783	ARG	2.0
1	D	817	ALA	2.0
1	B	741	HIS	2.0
1	B	749	VAL	2.0
1	A	936	ALA	2.0
1	C	815	TYR	2.0
1	C	784	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	HG9	B	451	24/25	0.27	3.29	37,49,69,70	0
3	HG9	A	453	24/25	0.26	3.19	42,53,65,67	0
3	HG9	B	452	24/25	0.25	1.89	48,54,68,70	0
4	666	C	463	30/30	0.20	0.98	39,53,72,85	0
2	MG	A	471	1/1	0.26	0.74	34,34,34,34	0
3	HG9	A	454	24/25	0.20	0.73	46,61,71,74	0
4	666	B	462	30/30	0.19	0.67	36,43,60,68	0
2	MG	B	473	1/1	0.27	0.54	23,23,23,23	0
2	MG	C	476	1/1	0.18	0.31	37,37,37,37	0
4	666	A	461	30/30	0.16	0.31	32,43,59,73	0
2	MG	A	472	1/1	0.17	0.01	32,32,32,32	0
4	666	D	464	30/30	0.17	-0.04	46,50,65,82	0
2	MG	B	474	1/1	0.16	-0.66	33,33,33,33	0
2	MG	D	477	1/1	0.18	-0.77	34,34,34,34	0
2	MG	D	478	1/1	0.13	-1.12	31,31,31,31	0
2	MG	A	479	1/1	0.06	-2.14	39,39,39,39	0
2	MG	C	475	1/1	0.14	-3.93	28,28,28,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.