



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:36 am GMT

PDB ID : 1SO2
Title : CATALYTIC DOMAIN OF HUMAN PHOSPHODIESTERASE 3B In COM-
PLEX WITH A DIHYDROPYRIDAZINE INHIBITOR
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M.R.
Deposited on : 2004-03-12
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

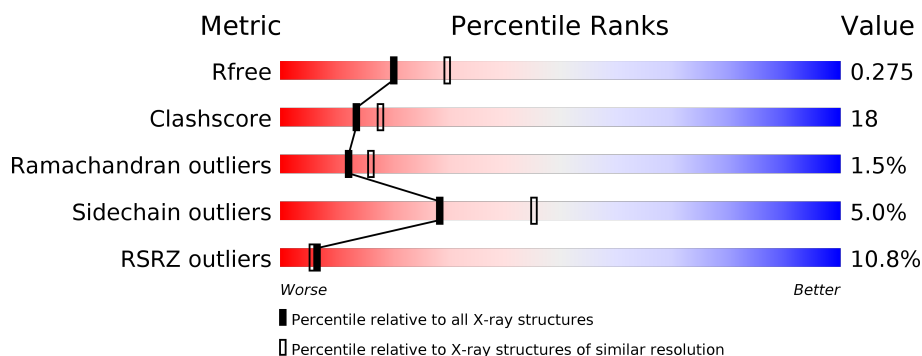
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	420	<div> <div>9%</div> <div> <div>61%</div> <div>23%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	420	<div> <div>8%</div> <div> <div>60%</div> <div>24%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	420	<div> <div>8%</div> <div> <div>63%</div> <div>24%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	420	<div> <div>13%</div> <div> <div>50%</div> <div>33%</div> <div>5%</div> <div>13%</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 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.

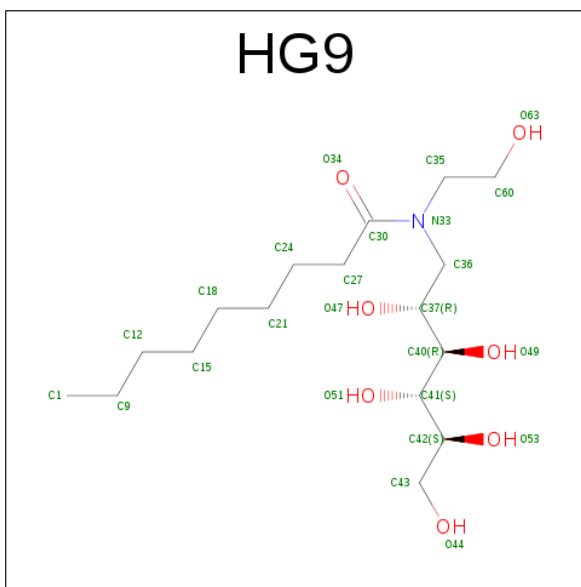
- Molecule 1 is a protein called cGMP-inhibited 3',5'-cyclic phosphodiesterase B.

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).

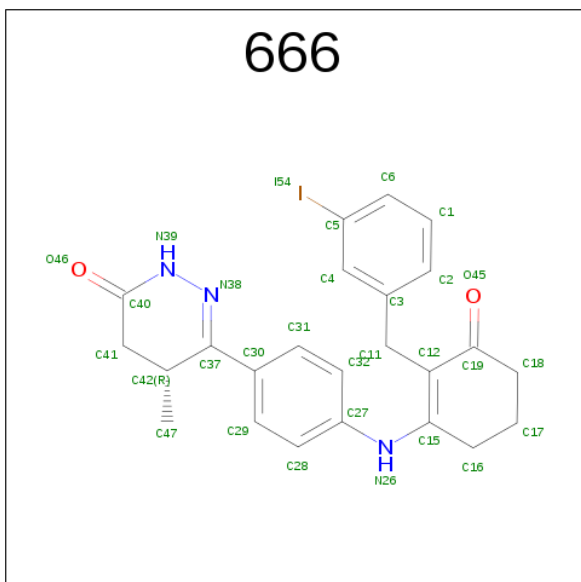
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	3	Total	Mg	0	0
			3	3		
2	D	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 1-DEOXY-1-[(2-HYDROXYETHYL)(NONANOYL)AMINO]HEXITOL (three-letter code: HG9) (formula: C₁₇H₃₅NO₇).



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: $C_{24}H_{24}IN_3O_2$).



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		

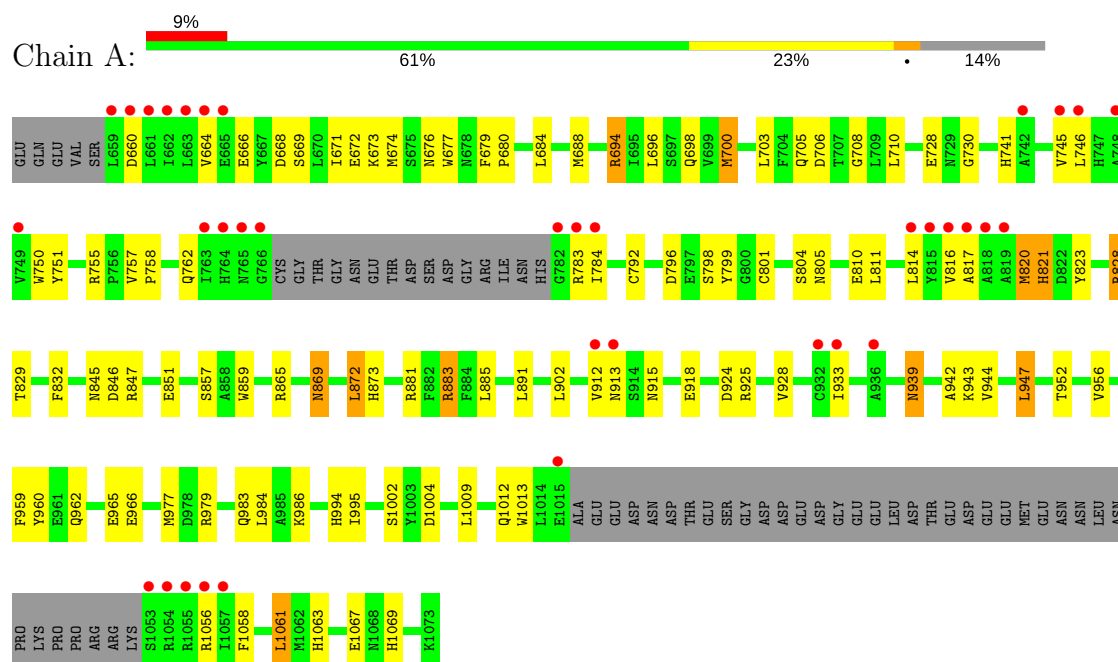
- Molecule 5 is water.

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		

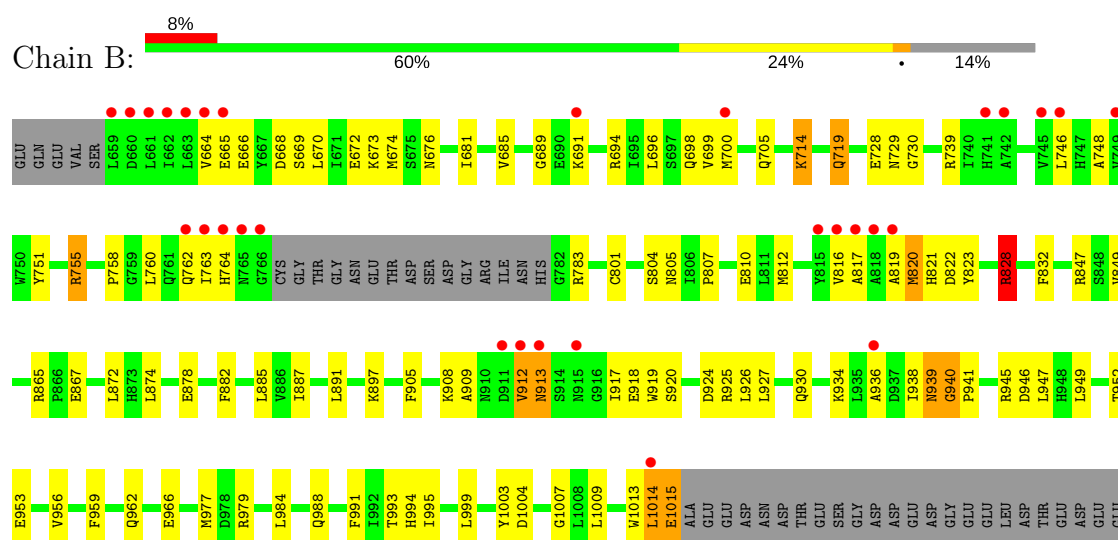
3 Residue-property plots

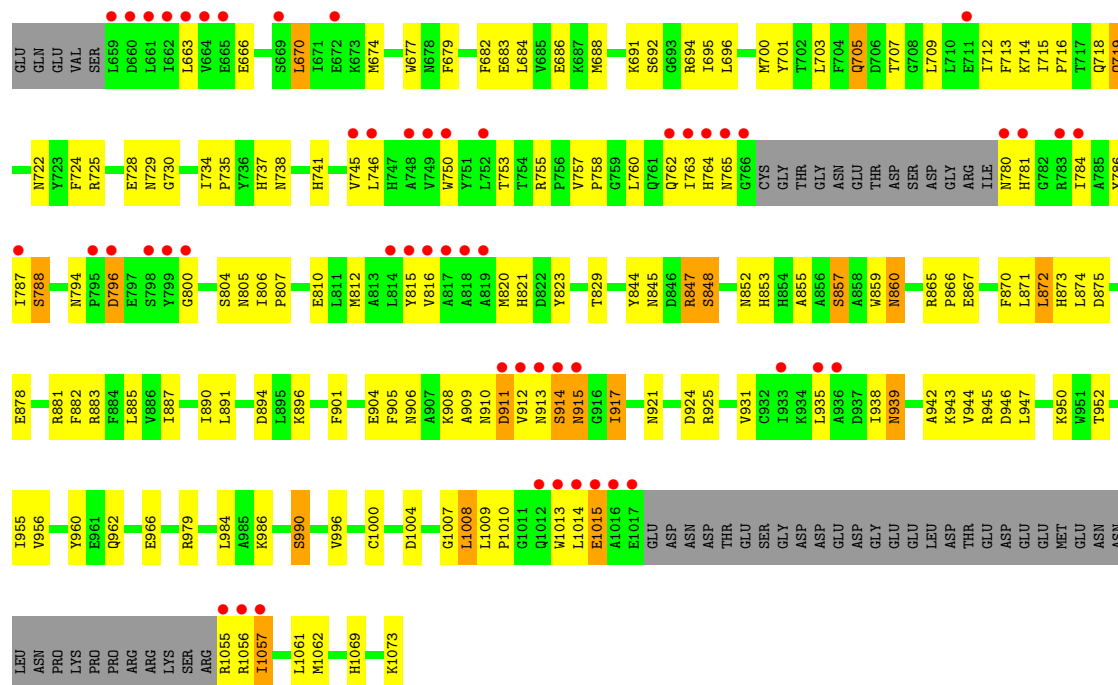
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.39Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.232 , 0.277 0.228 , 0.275	Depositor DCC
R_{free} test set	4345 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.881	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12292	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2916	0	2803	83	0
1	B	2909	0	2788	107	0
1	C	2964	0	2834	87	0
1	D	2916	0	2788	148	0
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 18.

All (419) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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:A:847:ARG:CZ	1:B:891:LEU:HD13	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:716:PRO:HB2	1:D:719:GLN:HE22	1.53	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:A:979:ARG:HH11	3:A:453:HG9:H602	1.53	0.71
1:B:991:PHE:HA	1:B:995:ILE:HD13	1.72	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:B:1069:HIS:NE2	1:B:1073:LYS:HD2	2.08	0.69
1:D:709:LEU:HD23	1:D:787:ILE:HD11	1.75	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:A:883:ARG:HH11	1:A:883:ARG:HG2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:960:TYR:HB3	1:C:979:ARG:NH2	2.11	0.65
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:A:1063:HIS:O	1:A:1067:GLU:HG3	1.98	0.64
1:D:804:SER:C	1:D:805:ASN:HD22	2.00	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: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:939:ASN:ND2	1:B:939:ASN:C	2.52	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
4:B:462:666:H28	4:B:462:666:H162	1.82	0.62
1:D:881:ARG:O	1:D:885:LEU:HD13	2.00	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:B:681:ILE:O	1:B:685:VAL:HG23	2.02	0.60
1:C:1013:TRP:CZ3	1:C:1055:ARG:HB3	2.37	0.60
1:D:865:ARG:HG2	1:D:865:ARG:NH1	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:730:GLY:HA3	1:B:823:TYR:CE1	2.39	0.58
1:B:939:ASN:HD22	1:B:940:GLY:N	2.02	0.58
1:B:917:ILE:HG23	1:B:924:ASP:HB3	1.85	0.58
1:D:716:PRO:CG	1:D:719:GLN:NE2	2.67	0.58
1:B:930:GLN:O	1:B:934:LYS:HG3	2.03	0.58
1:A:757:VAL:HG13	1:A:1009:LEU:O	2.04	0.58
1:D:719:GLN:NE2	1:D:719:GLN:H	2.01	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:A:730:GLY:HA3	1:A:823:TYR:HE1	1.69	0.57
1:B:1003:TYR:HD2	1:B:1009:LEU:HG	1.70	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:A:995:ILE:N	1:A:995:ILE:HD12	2.20	0.56
1:C:660:ASP:O	1:C:663:LEU:HB2	2.05	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:A:684:LEU:O	1:A:688:MET:HG3	2.05	0.56
1:D:812:MET:O	1:D:816:VAL:HG23	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:A:783:ARG:HG2	1:A:784:ILE:N	2.21	0.55
1:D:763:ILE:O	1:D:765:ASN:N	2.39	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:C:912:VAL:HG23	1:C:913:ASN:H	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:712:ILE:HD12	1:D:787:ILE:CD1	2.37	0.54
1:A:751:TYR:CZ	1:A:755:ARG:HG3	2.42	0.54
1:C:1061:LEU:C	1:C:1061:LEU:HD12	2.28	0.54
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:A:962:GLN:O	1:A:966:GLU:HG3	2.08	0.54
1:D:716:PRO:CB	1:D:719:GLN:NE2	2.71	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:A:708:GLY:HA2	5:A:128:HOH:O	2.07	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: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:A:783:ARG:HG2	1:A:784:ILE:H	1.72	0.53
1:D:716:PRO:HG2	1:D:719:GLN:HE21	1.74	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:A:952:THR:O	1:A:956:VAL:HG13	2.08	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: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: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:D:694:ARG:HA	1:D:728:GLU:OE1	2.08	0.52
1:A:817:ALA:O	1:A:821:HIS:HB3	2.10	0.52
1:B:926:LEU:O	1:B:930:GLN:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:696:LEU:HB3	1:B:728:GLU:HG2	1.93	0.50
1:D:986:LYS:O	1:D:990:SER:HB2	2.11	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:A:669:SER:O	1:A:673:LYS:HG3	2.12	0.50
1:B:817:ALA:O	1:B:821:HIS:HB3	2.11	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:1069:HIS:HE2	1:D:1073:LYS:HD3	1.76	0.49
1:D:763:ILE:C	1:D:765:ASN:N	2.65	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:B:666:GLU:O	1:B:669:SER:HB3	2.12	0.49
1:D:844:TYR:CE2	1:D:852:ASN:HB3	2.47	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:C:969:LEU:HB2	1:C:971:LEU:HD12	1.95	0.49
1:D:787:ILE:CG2	1:D:788:SER:N	2.76	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: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:D:913:ASN:O	1:D:915:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:912:VAL:C	1:D:914:SER:N	2.67	0.48
1:D:955:ILE:HG23	1:D:956:VAL:N	2.27	0.48
1:A:872:LEU:HD13	1:A:873:HIS:N	2.29	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:D:901:PHE:O	1:D:904:GLU:HB2	2.14	0.48
1:C:912:VAL:CG2	1:C:913:ASN:N	2.75	0.48
1:D:679:PHE:HZ	1:D:684:LEU:CD2	2.20	0.48
1:A:891:LEU:HD13	1:B:847:ARG:CZ	2.44	0.47
1:B:669:SER:O	1:B:672:GLU:HB3	2.14	0.47
1:D:855:ALA:HB2	1:D:890:ILE:HG21	1.95	0.47
1:D:881:ARG:CG	1:D:881:ARG:HH11	2.24	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:C:711:GLU:OE1	1:C:714:LYS:NZ	2.42	0.47
1:D:1004:ASP:CB	1:D:1009:LEU:HD12	2.44	0.47
1:D:917:ILE:HD12	1:D:924:ASP:HB3	1.96	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:C:846:ASP:OD2	1:D:883:ARG:NH1	2.45	0.47
1:D:1009:LEU:HD23	1:D:1010:PRO:HD2	1.97	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: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: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: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:B:938:ILE:HD11	1:B:999:LEU:HD23	1.96	0.46
1:C:1004:ASP:CB	1:C:1009:LEU:HD12	2.45	0.46
1:A:703:LEU:HD22	1:A:750:TRP:CE2	2.50	0.46
1:A:902:LEU:HD11	1:A:1002:SER:OG	2.15	0.46
1:B:994:HIS:HB2	1:B:995:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:LEU:HD11	1:A:933:ILE:HB	1.97	0.46
1:C:912:VAL:CG2	1:C:913:ASN:H	2.29	0.46
1:B:816:VAL:O	1:B:819:ALA:HB3	2.15	0.46
1:D:1007:GLY:C	1:D:1008:LEU:HD23	2.35	0.46
1:A:823:TYR:HE2	1:A:857:SER:HB3	1.80	0.46
1:D:716:PRO:HG2	1:D:719:GLN:NE2	2.31	0.46
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:B:762:GLN:OE1	1:B:762:GLN:HA	2.16	0.45
1:B:918:GLU:C	1:B:920:SER:H	2.20	0.45
1:C:695:ILE:O	1:C:699:VAL:HG23	2.15	0.45
1:D:845:ASN:O	1:D:847:ARG:HG3	2.15	0.45
1:D:715:ILE:HG23	1:D:870:PHE:HB2	1.97	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:691:LYS:HE2	1:D:691:LYS:HB3	1.83	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:HG2	1:B:783:ARG:HH11	1.82	0.45
1:A:851:GLU:HB3	1:A:891:LEU:HD23	1.99	0.45
1:A:944:VAL:HG12	1:A:947:LEU:HD22	1.99	0.45
1:A:960:TYR:HB3	1:A:979:ARG:CZ	2.47	0.45
1:C:729:ASN:HA	1:C:739:ARG:HH22	1.81	0.45
1:C:762:GLN:HA	1:C:805:ASN:HD21	1.82	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:C:851:GLU:OE1	1:C:894:ASP:HB2	2.17	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:A:758:PRO:HG3	1:A:799:TYR:CE2	2.51	0.44
1:A:869:ASN:ND2	1:A:872:LEU:HB3	2.33	0.44
1:B:804:SER:C	1:B:805:ASN:HD22	2.20	0.44
1:C:832:PHE:O	1:C:835:ALA:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:909:ALA:HB2	1:B:917:ILE:CD1	2.41	0.44
1:D:738:ASN:HB2	5:D:342:HOH:O	2.18	0.44
1:D:871:LEU:O	1:D:874:LEU:HB2	2.18	0.44
1:D:944:VAL:O	1:D:945:ARG:C	2.56	0.44
1:B:670:LEU:HA	1:B:673:LYS:NZ	2.32	0.44
1:C:847:ARG:O	1:C:848:SER:C	2.55	0.44
1:C:718:GLN:O	1:C:722:ASN:ND2	2.50	0.44
1:C:739:ARG:HG3	5:C:311:HOH:O	2.18	0.44
1:D:674:MET:HE1	1:D:703:LEU:HD21	2.00	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:C:915:ASN:O	1:C:916:GLY:O	2.37	0.43
1:D:712:ILE:HD12	1:D:787:ILE:HD11	2.00	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: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:C:670:LEU:CD2	1:C:674:MET:SD	3.07	0.43
1:B:694:ARG:O	1:B:698:GLN:HG2	2.19	0.43
1:D:757:VAL:HG13	1:D:1009:LEU:O	2.18	0.43
1:A:796:ASP:OD1	1:A:798:SER:OG	2.12	0.43
1:C:1060:GLN:O	1:C:1063:HIS:HB3	2.18	0.43
1:A:758:PRO:HG3	1:A:799:TYR:HE2	1.84	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:B:674:MET:CE	1:B:699:VAL:HG13	2.48	0.43
1:B:729:ASN:HA	1:B:739:ARG:HH22	1.82	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:812:MET:HG2	1:B:882:PHE:HE1	1.83	0.43
1:B:810:GLU:HG2	1:B:885:LEU:HD13	2.01	0.43
1:D:952:THR:O	1:D:956:VAL:HG13	2.19	0.43
1:A:994:HIS:HB2	1:A:995:ILE:HD12	2.00	0.42
1:D:700:MET:HE3	1:D:746:LEU:CD2	2.49	0.42
1:B:758:PRO:HB3	1:B:1013:TRP:CE2	2.55	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:A:811:LEU:HA	1:A:811:LEU:HD23	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:679:PHE:HD1	1:A:680:PRO:HD2	1.84	0.42
1:D:755:ARG:O	1:D:757:VAL:HG23	2.19	0.42
1:D:712:ILE:HD12	1:D:787:ILE:HD13	2.00	0.42
1:D:874:LEU:HG	1:D:878:GLU:OE2	2.19	0.42
1:D:1055:ARG:CG	1:D:1056:ARG:N	2.82	0.42
1:A:669:SER:O	1:A:672:GLU:HB3	2.19	0.42
1:B:941:PRO:HD3	4:B:462:666:C40	2.50	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
1:A:983:GLN:OE1	1:A:986:LYS:HD3	2.20	0.42
1:B:714:LYS:HE3	1:B:714:LYS:HA	2.02	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:865:ARG:HG3	1:B:865:ARG:HH11	1.84	0.42
1:A:758:PRO:HB3	1:A:1013:TRP:CE2	2.55	0.41
1:D:806:ILE:HA	1:D:807:PRO:HD2	1.93	0.41
1:A:956:VAL:HG11	1:A:984:LEU:HD13	2.01	0.41
1:B:691:LYS:HE3	1:B:694:ARG:HH21	1.85	0.41
1:B:812:MET:HG2	1:B:882:PHE:CE1	2.55	0.41
1:C:681:ILE:O	1:C:685:VAL:HG23	2.20	0.41
1:D:1062:MET:HB2	1:D:1062:MET:HE3	1.92	0.41
1:D:935:LEU:HD12	1:D:935:LEU:HA	1.92	0.41
1:B:959:PHE:HB3	1:B:977:MET:HG2	2.00	0.41
1:C:700:MET:HE3	1:C:746:LEU:HD13	2.00	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:D:939:ASN:HD22	1:D:943:LYS:HG2	1.86	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:A:671:ILE:HA	1:A:671:ILE:HD13	1.93	0.41
1:A:677:TRP:O	1:A:943:LYS:HE2	2.20	0.41
1:B:1007:GLY:HA2	5:B:251:HOH:O	2.21	0.41
1:B:1014:LEU:O	1:B:1015:GLU:CB	2.68	0.41
1:B:760:LEU:HD23	1:B:801:CYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:821:HIS:NE2	1:B:822:ASP:OD2	2.53	0.41
1:B:952:THR:HG23	1:B:988:GLN:NE2	2.35	0.41
1:C:952:THR:O	1:C:956:VAL:HG13	2.20	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:D:700:MET:HE3	1:D:746:LEU:HD22	2.02	0.41
1:A:845:ASN:O	1:A:846:ASP:HB2	2.21	0.41
1:C:674:MET:HE3	1:C:699:VAL:HG13	2.03	0.41
1:B:953:GLU:O	1:B:956:VAL:HG22	2.20	0.41
1:C:887:ILE:HD13	1:D:845:ASN:HB3	2.03	0.41
1:D:872:LEU:N	1:D:872:LEU:HD12	2.35	0.41
1:A:741:HIS:O	1:A:745:VAL:HG23	2.21	0.41
1:B:783:ARG:NH1	1:B:783:ARG:HG2	2.36	0.41
1:D:881:ARG:NH1	1:D:881:ARG:HG3	2.32	0.41
1:C:663:LEU:HD13	1:C:666:GLU:OE1	2.20	0.40
1:C:847:ARG:O	1:C:849:VAL:N	2.54	0.40
1:C:909:ALA:HB2	1:C:917:ILE:CD1	2.52	0.40
1:C:998:PRO:HA	5:C:424:HOH:O	2.21	0.40
1:D:683:GLU:O	1:D:686:GLU:HB3	2.20	0.40
1:D:942:ALA:HB1	1:D:1061:LEU:HB2	2.03	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:C:1057:ILE:HD12	1:C:1057:ILE:O	2.21	0.40
1:D:904:GLU:O	1:D:905:PHE:C	2.60	0.40
1:B:748:ALA:HB3	1:B:936:ALA:HB1	2.04	0.40
1:C:960:TYR:HB3	1:C:979:ARG:CZ	2.52	0.40
1:D:688:MET:HE2	1:D:691:LYS:O	2.21	0.40
1:A:674:MET:C	1:A:676:ASN:H	2.25	0.40
1:B:897:LYS:HE2	1:B:897:LYS:HB3	1.91	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%)	28	41
1	B	357/420 (85%)	325 (91%)	26 (7%)	6 (2%)	11	13
1	C	366/420 (87%)	336 (92%)	25 (7%)	5 (1%)	13	18
1	D	359/420 (86%)	319 (89%)	31 (9%)	9 (2%)	6	6
All	All	1439/1680 (86%)	1317 (92%)	100 (7%)	22 (2%)	12	16

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%)	25	40
1	B	308/370 (83%)	295 (96%)	13 (4%)	34	53
1	C	313/370 (85%)	301 (96%)	12 (4%)	38	58
1	D	308/370 (83%)	288 (94%)	20 (6%)	20	31
All	All	1239/1480 (84%)	1177 (95%)	62 (5%)	28	45

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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	1.47	4 (17%)	27,28,29	1.29	2 (7%)
3	HG9	A	454	-	23,23,24	1.68	5 (21%)	27,28,29	1.51	4 (14%)
4	666	A	461	-	33,33,33	3.89	25 (75%)	36,46,46	2.53	9 (25%)
3	HG9	B	451	-	23,23,24	1.81	5 (21%)	27,28,29	1.17	3 (11%)
3	HG9	B	452	-	23,23,24	1.42	3 (13%)	27,28,29	1.31	5 (18%)
4	666	B	462	-	33,33,33	3.80	22 (66%)	36,46,46	2.46	7 (19%)
4	666	C	463	-	33,33,33	3.83	24 (72%)	36,46,46	2.55	8 (22%)
4	666	D	464	-	33,33,33	3.89	25 (75%)	36,46,46	2.54	10 (27%)

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 (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	461	666	N39-N38	-4.21	1.27	1.38
4	C	463	666	N39-N38	-3.81	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	464	666	N39-N38	-3.54	1.29	1.38
4	B	462	666	N39-N38	-3.46	1.29	1.38
4	C	463	666	C27-N26	-3.38	1.35	1.41
4	A	461	666	C27-N26	-3.11	1.35	1.41
4	B	462	666	C27-N26	-2.48	1.36	1.41
4	D	464	666	C27-N26	-2.33	1.37	1.41
4	D	464	666	O45-C19	-2.15	1.18	1.23
4	A	461	666	O46-C40	-2.13	1.18	1.23
3	A	454	HG9	C30-N33	2.04	1.39	1.35
4	D	464	666	C28-C27	2.05	1.42	1.39
4	D	464	666	C11-C12	2.09	1.54	1.51
4	C	463	666	C17-C16	2.12	1.58	1.52
4	A	461	666	C28-C27	2.16	1.42	1.39
4	B	462	666	C32-C31	2.20	1.42	1.38
3	B	452	HG9	C36-C37	2.20	1.56	1.52
3	A	453	HG9	C36-N33	2.23	1.51	1.47
4	C	463	666	C18-C19	2.23	1.53	1.50
3	A	454	HG9	C37-C40	2.27	1.57	1.53
4	A	461	666	C5-I54	2.29	2.16	2.10
4	B	462	666	C17-C16	2.31	1.59	1.52
3	A	453	HG9	C30-N33	2.33	1.40	1.35
4	C	463	666	C32-C31	2.34	1.42	1.38
4	D	464	666	C6-C5	2.34	1.43	1.38
4	B	462	666	C28-C27	2.36	1.43	1.39
4	C	463	666	C28-C27	2.36	1.43	1.39
4	B	462	666	C11-C3	2.37	1.55	1.51
4	A	461	666	C17-C16	2.39	1.59	1.52
4	A	461	666	C40-N39	2.40	1.37	1.34
4	A	461	666	C29-C30	2.45	1.43	1.39
4	A	461	666	C6-C5	2.50	1.44	1.38
4	A	461	666	C41-C40	2.53	1.54	1.50
4	D	464	666	C1-C6	2.57	1.43	1.38
4	C	463	666	C6-C5	2.57	1.44	1.38
3	B	452	HG9	C30-N33	2.57	1.40	1.35
4	D	464	666	C1-C2	2.62	1.43	1.38
4	A	461	666	C1-C2	2.67	1.44	1.38
4	D	464	666	C17-C16	2.69	1.60	1.52
4	B	462	666	C18-C19	2.82	1.54	1.50
4	B	462	666	C29-C30	2.82	1.44	1.39
3	B	451	HG9	C37-C40	2.83	1.59	1.53
4	D	464	666	C29-C30	2.83	1.44	1.39
4	D	464	666	C18-C19	2.85	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	461	666	C32-C27	2.90	1.44	1.39
4	B	462	666	C31-C30	2.91	1.44	1.39
4	B	462	666	C41-C40	3.02	1.55	1.50
4	D	464	666	C11-C3	3.05	1.56	1.51
4	C	463	666	C11-C12	3.06	1.55	1.51
4	B	462	666	C32-C27	3.07	1.44	1.39
4	D	464	666	C32-C31	3.10	1.44	1.38
4	A	461	666	C32-C31	3.10	1.44	1.38
4	C	463	666	C29-C30	3.13	1.44	1.39
4	C	463	666	C32-C27	3.13	1.44	1.39
4	C	463	666	C1-C2	3.14	1.44	1.38
4	B	462	666	C1-C6	3.16	1.44	1.38
4	C	463	666	C41-C40	3.18	1.56	1.50
4	A	461	666	C18-C19	3.25	1.55	1.50
3	B	451	HG9	C36-N33	3.30	1.53	1.47
4	C	463	666	C1-C6	3.31	1.45	1.38
3	A	453	HG9	C36-C37	3.35	1.57	1.52
4	C	463	666	C31-C30	3.35	1.44	1.39
4	A	461	666	C31-C30	3.37	1.44	1.39
4	B	462	666	C4-C3	3.38	1.45	1.39
4	D	464	666	C41-C40	3.38	1.56	1.50
3	A	454	HG9	C36-N33	3.39	1.53	1.47
3	A	454	HG9	C36-C37	3.42	1.57	1.52
4	B	462	666	C1-C2	3.66	1.45	1.38
4	D	464	666	C31-C30	3.69	1.45	1.39
4	A	461	666	C2-C3	3.70	1.46	1.38
3	B	451	HG9	C30-N33	3.70	1.43	1.35
4	A	461	666	C1-C6	3.72	1.46	1.38
3	B	451	HG9	C27-C30	3.74	1.59	1.51
4	D	464	666	C32-C27	3.75	1.45	1.39
4	A	461	666	C4-C3	3.77	1.45	1.39
4	C	463	666	C2-C3	3.79	1.46	1.38
4	D	464	666	C2-C3	3.85	1.46	1.38
4	D	464	666	C4-C3	3.88	1.46	1.39
3	B	451	HG9	C36-C37	3.96	1.58	1.52
4	B	462	666	C42-C37	4.04	1.57	1.51
3	A	453	HG9	C27-C30	4.10	1.60	1.51
4	C	463	666	C42-C37	4.11	1.57	1.51
4	C	463	666	C11-C3	4.13	1.58	1.51
3	B	452	HG9	C27-C30	4.44	1.61	1.51
4	A	461	666	C42-C37	4.45	1.58	1.51
3	A	454	HG9	C27-C30	4.45	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	464	666	C19-C12	4.46	1.56	1.46
4	B	462	666	C2-C3	4.47	1.48	1.38
4	D	464	666	C42-C37	4.60	1.58	1.51
4	C	463	666	C16-C15	4.79	1.55	1.49
4	C	463	666	C4-C3	4.84	1.47	1.39
4	B	462	666	C16-C15	4.85	1.55	1.49
4	A	461	666	C16-C15	5.12	1.56	1.49
4	B	462	666	C19-C12	5.36	1.58	1.46
4	A	461	666	C19-C12	5.38	1.58	1.46
4	C	463	666	C19-C12	5.48	1.58	1.46
4	B	462	666	C4-C5	5.69	1.48	1.38
4	C	463	666	C17-C18	5.74	1.70	1.52
4	A	461	666	C17-C18	5.85	1.71	1.52
4	D	464	666	C16-C15	5.88	1.57	1.49
4	D	464	666	C17-C18	5.96	1.71	1.52
4	A	461	666	C4-C5	6.02	1.48	1.38
4	B	462	666	C17-C18	6.29	1.72	1.52
4	D	464	666	C4-C5	6.47	1.49	1.38
4	C	463	666	C4-C5	6.68	1.49	1.38
4	C	463	666	C37-N38	7.15	1.37	1.29
4	D	464	666	C37-N38	8.17	1.38	1.29
4	A	461	666	C37-N38	8.68	1.38	1.29
4	B	462	666	C37-N38	8.93	1.39	1.29
4	C	463	666	C15-N26	9.53	1.48	1.35
4	B	462	666	C15-N26	9.90	1.49	1.35
4	A	461	666	C15-N26	10.24	1.49	1.35
4	D	464	666	C15-N26	10.40	1.49	1.35

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	462	666	C11-C12-C19	-9.54	102.99	118.49
4	D	464	666	C11-C12-C19	-9.33	103.33	118.49
4	A	461	666	C11-C12-C19	-8.76	104.26	118.49
4	C	463	666	C19-C12-C15	-8.16	113.59	120.37
4	C	463	666	C11-C12-C19	-8.00	105.49	118.49
4	A	461	666	C19-C12-C15	-7.26	114.34	120.37
4	B	462	666	C19-C12-C15	-6.57	114.92	120.37
4	D	464	666	C19-C12-C15	-6.21	115.21	120.37
4	D	464	666	C12-C15-N26	-5.65	112.75	123.05
4	C	463	666	C12-C15-N26	-5.64	112.78	123.05
4	A	461	666	C12-C15-N26	-5.59	112.86	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	462	666	C12-C15-N26	-5.38	113.25	123.05
4	C	463	666	C6-C5-C4	-3.23	117.53	121.21
4	A	461	666	C6-C5-C4	-2.98	117.83	121.21
4	C	463	666	C18-C17-C16	-2.75	103.22	112.05
4	D	464	666	C3-C11-C12	-2.71	109.03	114.20
3	B	452	HG9	O53-C42-C43	-2.71	102.94	109.21
4	A	461	666	C18-C17-C16	-2.58	103.74	112.05
4	B	462	666	C18-C17-C16	-2.57	103.78	112.05
4	D	464	666	C6-C5-C4	-2.48	118.39	121.21
3	A	454	HG9	C35-N33-C30	-2.38	113.26	120.79
4	D	464	666	C18-C17-C16	-2.25	104.83	112.05
3	B	452	HG9	O44-C43-C42	-2.23	106.19	111.11
4	A	461	666	C29-C30-C37	-2.03	118.32	120.76
4	D	464	666	C4-C5-I54	2.01	121.99	119.35
3	B	452	HG9	C36-C37-C40	2.01	115.58	109.82
4	C	463	666	C17-C18-C19	2.03	117.04	113.52
3	B	451	HG9	C35-N33-C36	2.04	118.79	116.40
3	B	452	HG9	C60-C35-N33	2.10	117.76	112.38
3	B	451	HG9	C60-C35-N33	2.29	118.25	112.38
4	B	462	666	C17-C18-C19	2.33	117.56	113.52
4	A	461	666	C17-C18-C19	2.45	117.77	113.52
4	D	464	666	C17-C18-C19	2.67	118.14	113.52
4	B	462	666	C16-C15-N26	2.80	122.96	117.35
4	D	464	666	C16-C15-N26	2.84	123.04	117.35
3	B	452	HG9	C35-N33-C36	2.86	119.74	116.40
3	B	451	HG9	C36-C37-C40	2.88	118.05	109.82
4	A	461	666	C16-C15-N26	2.91	123.18	117.35
3	A	453	HG9	C35-N33-C36	2.92	119.81	116.40
4	C	463	666	C16-C15-N26	2.94	123.23	117.35
3	A	454	HG9	C60-C35-N33	3.15	120.45	112.38
3	A	454	HG9	C36-C37-C40	3.24	119.08	109.82
3	A	453	HG9	C60-C35-N33	3.43	121.17	112.38
4	C	463	666	C27-N26-C15	3.86	135.71	127.20
4	A	461	666	C27-N26-C15	3.88	135.73	127.20
4	B	462	666	C27-N26-C15	3.91	135.81	127.20
4	D	464	666	C27-N26-C15	4.20	136.44	127.20
3	A	454	HG9	C35-N33-C36	4.43	121.58	116.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	453	HG9	2	0
4	A	461	666	2	0
3	B	451	HG9	2	0
4	B	462	666	2	0
4	C	463	666	1	0
4	D	464	666	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	363/420 (86%)	0.28	36 (9%) 8 7	26, 42, 69, 77	0
1	B	363/420 (86%)	0.29	33 (9%) 10 9	23, 43, 70, 79	0
1	C	372/420 (88%)	0.40	35 (9%) 9 8	34, 49, 72, 78	0
1	D	365/420 (86%)	0.74	54 (14%) 3 2	33, 55, 74, 79	0
All	All	1463/1680 (87%)	0.43	158 (10%) 6 6	23, 48, 72, 79	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1016	ALA	9.9
1	C	661	LEU	7.8
1	A	662	ILE	7.7
1	A	659	LEU	7.2
1	A	1053	SER	7.0
1	B	659	LEU	7.0
1	C	664	VAL	6.9
1	B	662	ILE	6.6
1	D	912	VAL	6.5
1	D	662	ILE	6.4
1	B	660	ASP	6.1
1	A	661	LEU	6.0
1	A	764	HIS	6.0
1	B	661	LEU	5.9
1	D	659	LEU	5.8
1	A	766	GLY	5.6
1	C	662	ILE	5.6
1	A	1055	ARG	5.5
1	A	765	ASN	5.5
1	A	1054	ARG	5.4
1	D	1056	ARG	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	661	LEU	5.1
1	C	767	CYS	5.1
1	C	912	VAL	5.0
1	D	780	ASN	4.8
1	B	1055	ARG	4.8
1	C	665	GLU	4.8
1	C	765	ASN	4.8
1	D	795	PRO	4.7
1	D	660	ASP	4.7
1	D	1017	GLU	4.6
1	A	660	ASP	4.6
1	D	781	HIS	4.6
1	C	764	HIS	4.5
1	D	663	LEU	4.3
1	C	913	ASN	4.2
1	D	784	ILE	4.2
1	D	665	GLU	4.2
1	C	766	GLY	4.1
1	C	1054	ARG	4.0
1	D	749	VAL	4.0
1	B	912	VAL	4.0
1	C	1053	SER	3.8
1	C	663	LEU	3.8
1	D	748	ALA	3.8
1	A	749	VAL	3.8
1	B	764	HIS	3.7
1	C	914	SER	3.7
1	D	1055	ARG	3.7
1	D	914	SER	3.7
1	B	1053	SER	3.7
1	D	766	GLY	3.6
1	A	782	GLY	3.6
1	D	664	VAL	3.6
1	D	819	ALA	3.6
1	C	1015	GLU	3.6
1	D	764	HIS	3.6
1	B	663	LEU	3.6
1	D	815	TYR	3.6
1	C	780	ASN	3.6
1	C	779	ILE	3.5
1	A	663	LEU	3.5
1	A	783	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	749	VAL	3.5
1	D	1014	LEU	3.4
1	A	817	ALA	3.4
1	D	913	ASN	3.3
1	C	746	LEU	3.3
1	C	1056	ARG	3.3
1	A	933	ILE	3.3
1	B	765	ASN	3.3
1	C	659	LEU	3.3
1	D	1012	GLN	3.3
1	A	665	GLU	3.2
1	A	1056	ARG	3.2
1	D	745	VAL	3.2
1	C	1055	ARG	3.2
1	D	711	GLU	3.1
1	D	746	LEU	3.1
1	B	816	VAL	3.1
1	D	818	ALA	3.1
1	D	936	ALA	3.1
1	D	798	SER	3.1
1	B	766	GLY	3.1
1	A	748	ALA	3.0
1	D	765	ASN	3.0
1	B	818	ALA	3.0
1	C	748	ALA	2.9
1	A	818	ALA	2.9
1	B	819	ALA	2.9
1	D	816	VAL	2.9
1	B	762	GLN	2.9
1	A	784	ILE	2.9
1	D	1015	GLU	2.9
1	D	1057	ILE	2.9
1	B	817	ALA	2.9
1	A	816	VAL	2.8
1	B	745	VAL	2.8
1	C	936	ALA	2.8
1	A	913	ASN	2.8
1	A	932	CYS	2.7
1	D	1013	TRP	2.7
1	B	911	ASP	2.7
1	A	745	VAL	2.7
1	D	814	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	664	VAL	2.7
1	D	933	ILE	2.6
1	D	799	TYR	2.6
1	B	664	VAL	2.6
1	B	746	LEU	2.6
1	B	913	ASN	2.6
1	C	915	ASN	2.6
1	C	774	ASP	2.6
1	B	665	GLU	2.6
1	D	911	ASP	2.5
1	A	1015	GLU	2.5
1	D	915	ASN	2.5
1	B	936	ALA	2.5
1	A	815	TYR	2.5
1	D	817	ALA	2.5
1	C	776	ASP	2.5
1	C	783	ARG	2.4
1	B	1056	ARG	2.4
1	A	814	LEU	2.4
1	B	1014	LEU	2.4
1	D	935	LEU	2.4
1	D	762	GLN	2.4
1	C	782	GLY	2.4
1	C	763	ILE	2.4
1	D	750	TRP	2.4
1	A	912	VAL	2.4
1	B	691	LYS	2.4
1	C	815	TYR	2.4
1	B	741	HIS	2.3
1	B	700	MET	2.3
1	B	815	TYR	2.3
1	D	752	LEU	2.3
1	A	742	ALA	2.3
1	A	936	ALA	2.3
1	C	911	ASP	2.3
1	D	787	ILE	2.3
1	C	818	ALA	2.3
1	A	746	LEU	2.3
1	D	783	ARG	2.2
1	B	749	VAL	2.2
1	B	915	ASN	2.2
1	C	777	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	763	ILE	2.2
1	C	814	LEU	2.2
1	A	819	ALA	2.1
1	D	796	ASP	2.1
1	A	1057	ILE	2.1
1	D	763	ILE	2.1
1	D	672	GLU	2.1
1	A	763	ILE	2.1
1	B	742	ALA	2.0
1	D	669	SER	2.0
1	D	800	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	HG9	B	451	24/25	0.78	0.28	3.46	37,49,69,70	0
3	HG9	A	453	24/25	0.80	0.27	3.45	42,53,65,67	0
3	HG9	B	452	24/25	0.76	0.25	1.91	48,54,68,70	0
3	HG9	A	454	24/25	0.84	0.21	0.89	46,61,71,74	0
4	666	C	463	30/30	0.93	0.20	0.88	39,53,72,85	0
2	MG	A	471	1/1	0.99	0.27	0.67	34,34,34,34	0
4	666	B	462	30/30	0.95	0.20	0.55	36,43,60,68	0
2	MG	B	473	1/1	1.00	0.29	0.46	23,23,23,23	0
4	666	A	461	30/30	0.94	0.17	0.34	32,43,59,73	0
2	MG	A	472	1/1	0.96	0.19	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	666	D	464	30/30	0.95	0.18	-0.07	46,50,65,82	0
2	MG	C	476	1/1	0.97	0.17	-0.21	37,37,37,37	0
2	MG	D	477	1/1	0.99	0.18	-0.88	34,34,34,34	0
2	MG	D	478	1/1	0.99	0.13	-1.23	31,31,31,31	0
2	MG	B	474	1/1	0.97	0.14	-1.35	33,33,33,33	0
2	MG	C	475	1/1	0.99	0.15	-3.42	28,28,28,28	0
2	MG	A	479	1/1	0.97	0.06	-	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.