



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:12 PM GMT

PDB ID : 3T1I
Title : Crystal Structure of Human Mre11: Understanding Tumorigenic Mutations
Authors : Park, Y.B.; Chae, J.; Kim, Y.; Cho, Y.
Deposited on : 2011-07-22
Resolution : 3.00 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

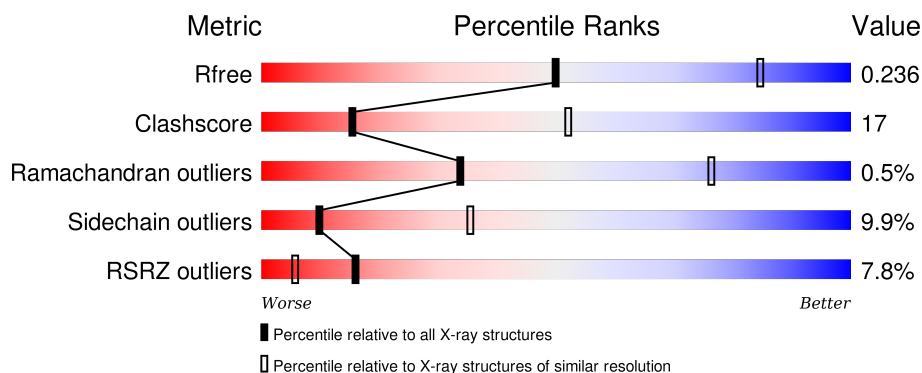
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	431	<div> <div>3%</div> <div>55%</div> <div>28%</div> <div>•</div> <div>13%</div> </div>
1	B	431	<div> <div>9%</div> <div>55%</div> <div>29%</div> <div>•</div> <div>12%</div> </div>
1	C	431	<div> <div>3%</div> <div>53%</div> <div>30%</div> <div>5%</div> <div>13%</div> </div>
1	D	431	<div> <div>12%</div> <div>54%</div> <div>31%</div> <div>•</div> <div>10%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DTT	A	452	-	-	X	X
4	GOL	A	458	-	-	-	X
4	GOL	C	453	-	-	-	X
4	GOL	C	454	-	-	-	X
4	GOL	C	455	-	-	-	X
4	GOL	C	456	-	-	-	X
4	GOL	D	452	-	-	-	X
4	GOL	D	453	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12407 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 Double-strand break repair protein MRE11A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	Se	0	0	0
			3032	1933	528	556	6	9			
1	B	378	Total	C	N	O	S	Se	0	0	0
			3045	1941	530	559	6	9			
1	C	377	Total	C	N	O	S	Se	0	0	0
			3038	1934	530	559	6	9			
1	D	386	Total	C	N	O	S	Se	0	0	0
			3112	1986	541	570	6	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	EXPRESSION TAG	UNP P49959
A	-18	GLY	-	EXPRESSION TAG	UNP P49959
A	-17	SER	-	EXPRESSION TAG	UNP P49959
A	-16	SER	-	EXPRESSION TAG	UNP P49959
A	-15	HIS	-	EXPRESSION TAG	UNP P49959
A	-14	HIS	-	EXPRESSION TAG	UNP P49959
A	-13	HIS	-	EXPRESSION TAG	UNP P49959
A	-12	HIS	-	EXPRESSION TAG	UNP P49959
A	-11	HIS	-	EXPRESSION TAG	UNP P49959
A	-10	HIS	-	EXPRESSION TAG	UNP P49959
A	-9	SER	-	EXPRESSION TAG	UNP P49959
A	-8	SER	-	EXPRESSION TAG	UNP P49959
A	-7	GLY	-	EXPRESSION TAG	UNP P49959
A	-6	LEU	-	EXPRESSION TAG	UNP P49959
A	-5	VAL	-	EXPRESSION TAG	UNP P49959
A	-4	PRO	-	EXPRESSION TAG	UNP P49959
A	-3	ARG	-	EXPRESSION TAG	UNP P49959
A	-2	GLY	-	EXPRESSION TAG	UNP P49959
A	-1	SER	-	EXPRESSION TAG	UNP P49959
A	0	HIS	-	EXPRESSION TAG	UNP P49959
B	-19	MSE	-	EXPRESSION TAG	UNP P49959

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP P49959
B	-17	SER	-	EXPRESSION TAG	UNP P49959
B	-16	SER	-	EXPRESSION TAG	UNP P49959
B	-15	HIS	-	EXPRESSION TAG	UNP P49959
B	-14	HIS	-	EXPRESSION TAG	UNP P49959
B	-13	HIS	-	EXPRESSION TAG	UNP P49959
B	-12	HIS	-	EXPRESSION TAG	UNP P49959
B	-11	HIS	-	EXPRESSION TAG	UNP P49959
B	-10	HIS	-	EXPRESSION TAG	UNP P49959
B	-9	SER	-	EXPRESSION TAG	UNP P49959
B	-8	SER	-	EXPRESSION TAG	UNP P49959
B	-7	GLY	-	EXPRESSION TAG	UNP P49959
B	-6	LEU	-	EXPRESSION TAG	UNP P49959
B	-5	VAL	-	EXPRESSION TAG	UNP P49959
B	-4	PRO	-	EXPRESSION TAG	UNP P49959
B	-3	ARG	-	EXPRESSION TAG	UNP P49959
B	-2	GLY	-	EXPRESSION TAG	UNP P49959
B	-1	SER	-	EXPRESSION TAG	UNP P49959
B	0	HIS	-	EXPRESSION TAG	UNP P49959
C	-19	MSE	-	EXPRESSION TAG	UNP P49959
C	-18	GLY	-	EXPRESSION TAG	UNP P49959
C	-17	SER	-	EXPRESSION TAG	UNP P49959
C	-16	SER	-	EXPRESSION TAG	UNP P49959
C	-15	HIS	-	EXPRESSION TAG	UNP P49959
C	-14	HIS	-	EXPRESSION TAG	UNP P49959
C	-13	HIS	-	EXPRESSION TAG	UNP P49959
C	-12	HIS	-	EXPRESSION TAG	UNP P49959
C	-11	HIS	-	EXPRESSION TAG	UNP P49959
C	-10	HIS	-	EXPRESSION TAG	UNP P49959
C	-9	SER	-	EXPRESSION TAG	UNP P49959
C	-8	SER	-	EXPRESSION TAG	UNP P49959
C	-7	GLY	-	EXPRESSION TAG	UNP P49959
C	-6	LEU	-	EXPRESSION TAG	UNP P49959
C	-5	VAL	-	EXPRESSION TAG	UNP P49959
C	-4	PRO	-	EXPRESSION TAG	UNP P49959
C	-3	ARG	-	EXPRESSION TAG	UNP P49959
C	-2	GLY	-	EXPRESSION TAG	UNP P49959
C	-1	SER	-	EXPRESSION TAG	UNP P49959
C	0	HIS	-	EXPRESSION TAG	UNP P49959
D	-19	MSE	-	EXPRESSION TAG	UNP P49959
D	-18	GLY	-	EXPRESSION TAG	UNP P49959
D	-17	SER	-	EXPRESSION TAG	UNP P49959

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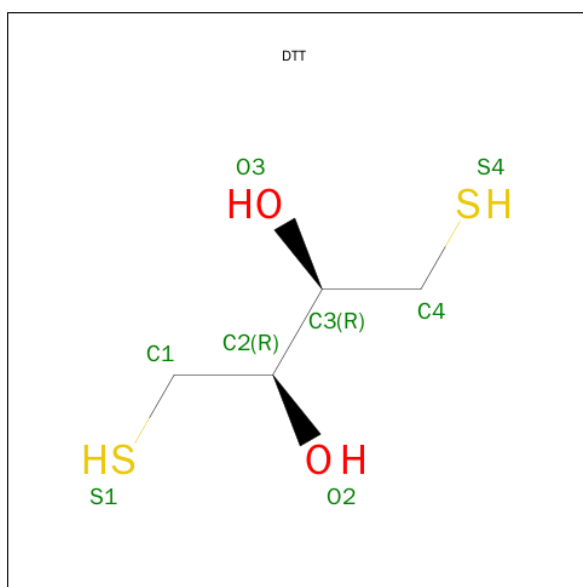
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP P49959
D	-15	HIS	-	EXPRESSION TAG	UNP P49959
D	-14	HIS	-	EXPRESSION TAG	UNP P49959
D	-13	HIS	-	EXPRESSION TAG	UNP P49959
D	-12	HIS	-	EXPRESSION TAG	UNP P49959
D	-11	HIS	-	EXPRESSION TAG	UNP P49959
D	-10	HIS	-	EXPRESSION TAG	UNP P49959
D	-9	SER	-	EXPRESSION TAG	UNP P49959
D	-8	SER	-	EXPRESSION TAG	UNP P49959
D	-7	GLY	-	EXPRESSION TAG	UNP P49959
D	-6	LEU	-	EXPRESSION TAG	UNP P49959
D	-5	VAL	-	EXPRESSION TAG	UNP P49959
D	-4	PRO	-	EXPRESSION TAG	UNP P49959
D	-3	ARG	-	EXPRESSION TAG	UNP P49959
D	-2	GLY	-	EXPRESSION TAG	UNP P49959
D	-1	SER	-	EXPRESSION TAG	UNP P49959
D	0	HIS	-	EXPRESSION TAG	UNP P49959

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

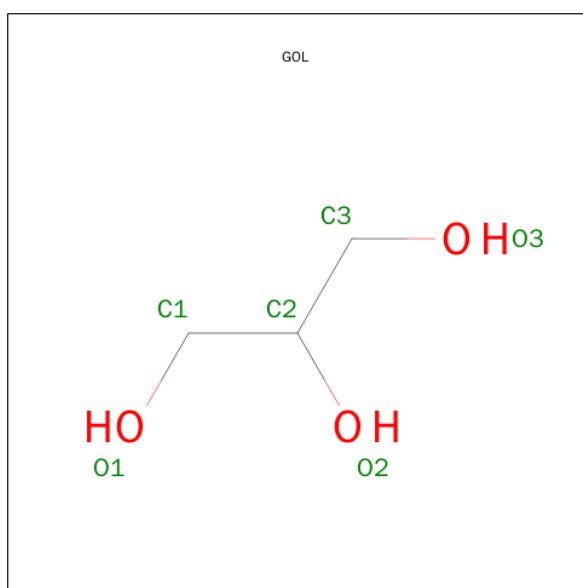
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mn 2 2	0	0
2	A	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		
3	A	1	Total	C	O	S	0	0
			8	4	2	2		

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



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total 22	O 22	0	0
5	B	11	Total 11	O 11	0	0
5	C	23	Total 23	O 23	0	0
5	D	10	Total 10	O 10	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.79Å 135.21Å 135.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.53 – 3.00 47.83 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.53-3.00) 93.7 (47.83-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.227 , 0.250 0.212 , 0.236	Depositor DCC
R_{free} test set	2350 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.8	EDS
Estimated twinning fraction	0.010 for -h,l,k 0.009 for -l,-k,-h 0.014 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 49966 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12407	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.49	0/3091	0.64	2/4158 (0.0%)
1	B	0.49	0/3104	0.64	1/4176 (0.0%)
1	C	0.48	0/3097	0.63	1/4166 (0.0%)
1	D	0.50	0/3175	0.64	0/4271
All	All	0.49	0/12467	0.64	4/16771 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	60	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	202	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	202	ARG	NE-CZ-NH1	5.27	122.94	120.30

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	3032	0	3013	94	0
1	B	3045	0	3027	100	0
1	C	3038	0	3013	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3112	0	3083	125	0
2	A	2	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	16	0	20	4	0
4	A	36	0	48	1	0
4	C	36	0	48	10	0
4	D	18	0	24	1	0
5	A	22	0	0	1	0
5	B	11	0	0	1	0
5	C	23	0	0	3	0
5	D	10	0	0	1	0
All	All	12407	0	12276	425	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 17.

All (425) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:VAL:HG13	1:B:278:GLU:HG2	1.31	1.09
1:C:271:VAL:HG13	1:C:278:GLU:HG2	1.37	1.07
1:D:271:VAL:HG13	1:D:278:GLU:HG2	1.30	1.06
1:A:271:VAL:HG13	1:A:278:GLU:HG2	1.30	1.06
1:C:159:VAL:HG13	1:D:159:VAL:HG13	1.07	1.04
1:D:103:PHE:HZ	1:D:146:CYS:HA	1.21	1.04
1:C:202:ARG:HH11	1:C:202:ARG:HG2	1.19	1.01
1:C:159:VAL:HG13	1:D:159:VAL:CG1	1.95	0.96
1:A:202:ARG:HH11	1:A:202:ARG:HG2	1.32	0.95
1:C:159:VAL:HG22	1:D:159:VAL:HG22	1.49	0.94
1:C:159:VAL:CG1	1:D:159:VAL:HG13	1.97	0.94
1:D:96:ASP:HA	1:D:97:GLN:HB3	1.47	0.94
1:D:202:ARG:HG2	1:D:202:ARG:HH11	1.32	0.92
1:D:103:PHE:CZ	1:D:146:CYS:HA	2.04	0.91
1:B:224:GLY:H	1:B:227:ASN:HB2	1.36	0.91
1:A:224:GLY:H	1:A:227:ASN:HB2	1.38	0.88
1:D:128:ASN:OD1	1:D:129:HIS:HD2	1.54	0.88
1:D:224:GLY:H	1:D:227:ASN:HB2	1.39	0.88
1:C:224:GLY:H	1:C:227:ASN:HB2	1.38	0.88
1:B:202:ARG:HH11	1:B:202:ARG:HG2	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLU:O	1:A:192:MSE:HE1	1.75	0.85
1:B:160:GLU:O	1:B:192:MSE:HE1	1.76	0.85
1:B:93:ILE:HD12	1:B:98:SER:HB2	1.59	0.84
1:C:160:GLU:O	1:C:192:MSE:HE1	1.79	0.83
1:D:160:GLU:O	1:D:192:MSE:HE1	1.79	0.82
1:A:159:VAL:HG13	1:B:159:VAL:HG13	1.61	0.82
1:C:202:ARG:HH11	1:C:202:ARG:CG	1.93	0.81
1:C:128:ASN:N	1:C:128:ASN:OD1	2.12	0.78
1:C:306:GLN:HA	4:C:453:GOL:H12	1.65	0.77
1:C:96:ASP:N	1:C:96:ASP:OD1	2.18	0.76
1:B:72:LEU:HD21	1:B:143:ILE:HG21	1.68	0.75
1:D:100:ASN:O	1:D:101:PHE:HB3	1.85	0.75
1:C:115:ASN:N	1:C:115:ASN:HD22	1.82	0.75
1:D:202:ARG:HH11	1:D:202:ARG:CG	2.00	0.74
1:A:72:LEU:HD21	1:A:143:ILE:HG21	1.70	0.74
1:B:128:ASN:OD1	1:B:128:ASN:N	2.21	0.74
1:A:39:THR:HG21	1:A:269:SER:HB2	1.70	0.74
1:B:189:LEU:HD23	1:B:229:ILE:CD1	2.18	0.74
1:C:11:ASN:O	1:C:174:THR:HG21	1.87	0.73
1:C:72:LEU:HD21	1:C:143:ILE:HG21	1.70	0.73
1:D:359:GLU:O	1:D:361:PRO:HD3	1.88	0.73
1:A:312:ILE:HD12	1:A:365:LEU:HD21	1.70	0.72
1:D:189:LEU:HD23	1:D:229:ILE:CD1	2.20	0.71
1:B:39:THR:HG21	1:B:269:SER:HB2	1.70	0.71
1:C:115:ASN:ND2	1:C:115:ASN:N	2.38	0.71
1:D:302:HIS:CD2	5:D:507:HOH:O	2.44	0.71
1:B:11:ASN:O	1:B:174:THR:HG21	1.91	0.71
1:A:202:ARG:HH11	1:A:202:ARG:CG	2.03	0.70
1:B:312:ILE:HD12	1:B:365:LEU:HD21	1.72	0.70
1:B:359:GLU:O	1:B:361:PRO:HD3	1.91	0.70
1:A:252:ALA:H	3:A:452:DTT:H12	1.54	0.70
1:A:128:ASN:OD1	1:A:128:ASN:N	2.20	0.70
1:D:39:THR:HG21	1:D:269:SER:HB2	1.73	0.70
1:D:312:ILE:HD12	1:D:365:LEU:HD21	1.72	0.69
1:C:11:ASN:O	1:C:174:THR:CG2	2.40	0.69
1:D:72:LEU:HD21	1:D:143:ILE:HG21	1.74	0.69
1:A:189:LEU:HD23	1:A:229:ILE:CD1	2.22	0.69
1:C:158:SER:HB3	1:C:161:LYS:O	1.93	0.69
1:C:312:ILE:HD12	1:C:365:LEU:HD21	1.73	0.68
1:B:202:ARG:HH11	1:B:202:ARG:CG	2.06	0.68
1:D:202:ARG:NH1	1:D:202:ARG:HG2	2.05	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LYS:HA	3:A:452:DTT:H11	1.75	0.68
1:A:11:ASN:O	1:A:174:THR:HG21	1.93	0.68
1:C:202:ARG:NH1	1:C:202:ARG:HG2	1.95	0.67
1:A:96:ASP:N	1:A:96:ASP:OD1	2.27	0.67
1:B:224:GLY:N	1:B:227:ASN:HB2	2.08	0.67
1:B:96:ASP:N	1:B:96:ASP:OD2	2.24	0.67
1:C:39:THR:HG21	1:C:269:SER:HB2	1.75	0.67
1:A:224:GLY:N	1:A:227:ASN:HB2	2.09	0.67
1:C:359:GLU:O	1:C:361:PRO:HD3	1.95	0.67
1:B:158:SER:HB3	1:B:161:LYS:O	1.95	0.67
1:B:253:PRO:HD3	1:B:296:MSE:HG2	1.76	0.66
1:C:224:GLY:N	1:C:227:ASN:HB2	2.09	0.66
1:B:11:ASN:O	1:B:174:THR:CG2	2.43	0.66
1:D:11:ASN:O	1:D:174:THR:HG21	1.95	0.66
1:B:283:HIS:CD2	1:B:300:PRO:HA	2.31	0.65
1:B:364:ARG:HG3	1:B:365:LEU:N	2.12	0.65
1:C:189:LEU:HD23	1:C:229:ILE:CD1	2.26	0.65
1:D:37:PHE:CD1	1:D:74:THR:HG21	2.32	0.65
1:A:158:SER:HB3	1:A:161:LYS:O	1.96	0.65
1:A:364:ARG:HG3	1:A:365:LEU:N	2.11	0.65
1:A:325:ASN:HB3	1:A:328:VAL:HB	1.78	0.65
1:D:253:PRO:HD3	1:D:296:MSE:HG2	1.78	0.64
1:D:158:SER:HB3	1:D:161:LYS:O	1.97	0.64
1:D:11:ASN:O	1:D:174:THR:CG2	2.46	0.64
1:B:380:ARG:O	1:B:384:LYS:HG3	1.98	0.64
1:B:189:LEU:HD23	1:B:229:ILE:HD11	1.79	0.64
1:B:325:ASN:HB3	1:B:328:VAL:HB	1.78	0.64
1:B:337:LEU:O	1:B:341:GLU:HB2	1.98	0.63
1:D:224:GLY:N	1:D:227:ASN:HB2	2.11	0.63
1:D:93:ILE:CD1	1:D:99:VAL:HG11	2.28	0.63
1:C:253:PRO:HD3	1:C:296:MSE:HG2	1.79	0.63
1:D:337:LEU:O	1:D:341:GLU:HB2	1.99	0.63
1:C:364:ARG:HG3	1:C:365:LEU:N	2.13	0.63
1:D:283:HIS:CD2	1:D:300:PRO:HA	2.34	0.62
1:D:103:PHE:O	1:D:103:PHE:CD1	2.52	0.62
1:C:98:SER:HB3	1:C:151:ASN:OD1	1.99	0.62
1:A:359:GLU:O	1:A:361:PRO:HD3	2.00	0.62
1:D:380:ARG:O	1:D:384:LYS:HG3	2.00	0.62
1:D:317:HIS:HB3	1:D:320:ILE:HD13	1.82	0.61
1:D:364:ARG:HG3	1:D:365:LEU:N	2.14	0.61
1:C:247:HIS:H	4:C:456:GOL:H12	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:LEU:HD12	1:C:369:TYR:HA	1.81	0.61
1:C:380:ARG:O	1:C:384:LYS:HG3	2.00	0.61
1:B:202:ARG:NH1	1:B:202:ARG:HG2	2.14	0.61
1:C:325:ASN:HB3	1:C:328:VAL:HB	1.81	0.61
1:D:369:TYR:HB2	1:D:373:PHE:HB2	1.82	0.61
1:D:325:ASN:HB3	1:D:328:VAL:HB	1.81	0.61
1:A:202:ARG:HG2	1:A:202:ARG:NH1	2.07	0.61
1:D:305:ARG:NH2	1:D:358:PRO:HB2	2.15	0.61
1:B:317:HIS:HB3	1:B:320:ILE:HD13	1.82	0.61
1:A:11:ASN:O	1:A:174:THR:CG2	2.49	0.61
1:A:18:ALA:O	1:A:57:LEU:HA	2.00	0.60
1:C:8:ASP:OD1	1:C:290:LYS:NZ	2.34	0.60
1:A:380:ARG:O	1:A:384:LYS:HG3	2.00	0.60
1:C:369:TYR:HB2	1:C:373:PHE:HB2	1.83	0.60
1:D:314:LEU:HD12	1:D:369:TYR:HA	1.83	0.60
1:A:317:HIS:HB3	1:A:320:ILE:HD13	1.82	0.60
1:D:189:LEU:HD23	1:D:229:ILE:HD11	1.82	0.60
1:B:18:ALA:O	1:B:57:LEU:HA	2.02	0.60
1:B:305:ARG:NH2	1:B:358:PRO:HB2	2.17	0.59
1:D:184:ILE:HG23	1:D:185:PRO:HD2	1.84	0.59
1:A:349:ARG:O	1:A:352:LEU:HB2	2.02	0.59
1:B:349:ARG:O	1:B:352:LEU:HB2	2.02	0.59
1:A:253:PRO:HD3	1:A:296:MSE:HG2	1.83	0.59
1:A:8:ASP:OD1	1:A:290:LYS:NZ	2.35	0.59
1:B:366:ARG:HG2	1:B:399:PHE:HE1	1.67	0.59
1:D:128:ASN:OD1	1:D:129:HIS:N	2.35	0.59
1:B:374:GLU:HG2	1:B:375:PRO:HD2	1.85	0.59
1:B:389:VAL:HG13	1:B:391:ASN:H	1.67	0.59
1:A:337:LEU:O	1:A:341:GLU:HB2	2.02	0.59
1:B:369:TYR:HB2	1:B:373:PHE:HB2	1.83	0.58
1:A:382:SER:O	1:A:386:VAL:HG23	2.02	0.58
1:A:389:VAL:HG13	1:A:391:ASN:H	1.69	0.58
1:D:366:ARG:HG2	1:D:399:PHE:HE1	1.67	0.58
1:A:369:TYR:HB2	1:A:373:PHE:HB2	1.84	0.58
1:D:26:MSE:O	1:D:33:GLY:HA2	2.03	0.58
1:B:236:ASP:HB3	1:B:259:GLN:HE21	1.68	0.58
1:C:374:GLU:HG2	1:C:375:PRO:HD2	1.85	0.58
1:A:366:ARG:HG2	1:A:399:PHE:HE1	1.67	0.58
1:C:337:LEU:O	1:C:341:GLU:HB2	2.03	0.58
1:A:236:ASP:HB3	1:A:259:GLN:HE21	1.68	0.58
1:B:314:LEU:HD12	1:B:369:TYR:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:ARG:O	1:C:352:LEU:HB2	2.03	0.58
1:C:317:HIS:HB3	1:C:320:ILE:HD13	1.86	0.58
1:A:37:PHE:CD1	1:A:74:THR:HG21	2.38	0.57
1:A:184:ILE:HG23	1:A:185:PRO:HD2	1.85	0.57
1:B:284:VAL:HG23	1:B:301:LEU:HD11	1.86	0.57
1:B:26:MSE:O	1:B:33:GLY:HA2	2.05	0.57
1:C:389:VAL:HG13	1:C:391:ASN:H	1.69	0.57
1:D:374:GLU:HG2	1:D:375:PRO:HD2	1.86	0.57
1:A:20:ASP:N	1:A:20:ASP:OD1	2.38	0.57
1:B:37:PHE:CD1	1:B:74:THR:HG21	2.39	0.57
1:D:349:ARG:O	1:D:352:LEU:HB2	2.05	0.57
1:D:236:ASP:HB3	1:D:259:GLN:HE21	1.69	0.57
1:D:305:ARG:HA	1:D:358:PRO:HG2	1.87	0.56
1:B:184:ILE:HG23	1:B:185:PRO:HD2	1.87	0.56
1:C:247:HIS:HB2	4:C:456:GOL:H12	1.86	0.56
1:A:374:GLU:HG2	1:A:375:PRO:HD2	1.87	0.56
1:A:284:VAL:HG23	1:A:301:LEU:HD11	1.87	0.56
1:B:271:VAL:CG1	1:B:278:GLU:HG2	2.21	0.55
1:C:283:HIS:CD2	1:C:300:PRO:HA	2.41	0.55
1:C:382:SER:O	1:C:386:VAL:HG23	2.06	0.55
1:B:131:ASP:HB2	1:B:132:PRO:CD	2.37	0.55
1:A:314:LEU:HD12	1:A:369:TYR:HA	1.88	0.55
1:A:305:ARG:NH2	1:A:358:PRO:HB2	2.21	0.55
1:A:131:ASP:HB2	1:A:132:PRO:CD	2.36	0.55
1:B:259:GLN:O	1:B:260:LEU:HB2	2.05	0.55
1:C:366:ARG:HG2	1:C:399:PHE:HE1	1.71	0.55
1:D:389:VAL:HG13	1:D:391:ASN:H	1.71	0.55
1:D:20:ASP:OD1	1:D:20:ASP:N	2.40	0.55
1:D:271:VAL:CG1	1:D:278:GLU:HG2	2.20	0.55
1:A:218:GLN:O	1:A:245:HIS:HB3	2.07	0.55
1:A:189:LEU:HD23	1:A:229:ILE:HD11	1.87	0.54
1:A:26:MSE:O	1:A:33:GLY:HA2	2.07	0.54
1:B:8:ASP:OD1	1:B:290:LYS:NZ	2.39	0.54
1:A:86:ASP:OD1	1:D:69:ARG:CG	2.56	0.54
1:C:184:ILE:HG23	1:C:185:PRO:HD2	1.88	0.54
1:D:128:ASN:OD1	1:D:129:HIS:CD2	2.46	0.54
1:C:37:PHE:CD1	1:C:74:THR:HG21	2.42	0.54
1:C:189:LEU:HD23	1:C:229:ILE:HD11	1.90	0.54
1:A:80:ARG:O	1:A:84:MSE:HG3	2.07	0.54
1:D:8:ASP:OD1	1:D:290:LYS:NZ	2.41	0.54
1:A:305:ARG:HA	1:A:358:PRO:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ILE:HG22	1:B:153:PHE:O	2.08	0.54
1:C:305:ARG:HA	1:C:358:PRO:HG2	1.90	0.54
1:D:96:ASP:HA	1:D:97:GLN:CB	2.20	0.53
1:C:284:VAL:HG23	1:C:301:LEU:HD11	1.90	0.53
1:C:131:ASP:HB2	1:C:132:PRO:CD	2.38	0.53
1:A:252:ALA:HB3	3:A:452:DTT:H12	1.91	0.53
1:D:284:VAL:HG23	1:D:301:LEU:HD11	1.91	0.53
1:C:125:ILE:HG22	1:C:153:PHE:O	2.08	0.53
1:D:382:SER:O	1:D:386:VAL:HG23	2.08	0.53
1:C:132:PRO:HA	1:C:138:LEU:O	2.09	0.53
1:B:382:SER:O	1:B:386:VAL:HG23	2.09	0.53
1:C:305:ARG:NH2	1:C:358:PRO:HB2	2.22	0.53
1:D:131:ASP:HB2	1:D:132:PRO:CD	2.39	0.53
1:D:35:ASP:OD1	1:D:305:ARG:NH1	2.42	0.53
1:C:35:ASP:OD1	1:C:305:ARG:NH1	2.42	0.53
1:D:18:ALA:O	1:D:57:LEU:HA	2.08	0.52
1:D:218:GLN:O	1:D:245:HIS:HB3	2.09	0.52
1:D:132:PRO:HA	1:D:138:LEU:O	2.10	0.52
1:A:271:VAL:HG22	1:A:278:GLU:HG3	1.91	0.52
1:A:125:ILE:HG22	1:A:153:PHE:O	2.09	0.52
1:C:26:MSE:O	1:C:33:GLY:HA2	2.09	0.52
1:B:218:GLN:O	1:B:245:HIS:HB3	2.10	0.52
1:A:271:VAL:CG1	1:A:278:GLU:HG2	2.21	0.51
1:A:286:LEU:C	1:A:286:LEU:HD12	2.30	0.51
1:D:101:PHE:C	1:D:101:PHE:CD1	2.82	0.51
1:D:128:ASN:ND2	1:D:245:HIS:CE1	2.78	0.51
1:A:35:ASP:OD1	1:A:305:ARG:NH1	2.43	0.51
1:A:262:TYR:N	1:A:262:TYR:CD2	2.78	0.51
1:A:238:ILE:O	1:A:261:PHE:HB3	2.10	0.51
1:B:36:THR:HG22	1:B:270:VAL:HG21	1.93	0.51
1:B:333:GLN:OE1	1:B:380:ARG:HD3	2.11	0.51
1:D:351:ARG:HG2	1:D:357:GLN:NE2	2.26	0.51
1:C:271:VAL:HG22	1:C:278:GLU:HG3	1.93	0.51
1:A:333:GLN:OE1	1:A:380:ARG:HD3	2.10	0.51
1:B:305:ARG:HA	1:B:358:PRO:HG2	1.91	0.51
1:C:351:ARG:HG2	1:C:357:GLN:NE2	2.26	0.51
1:B:211:PHE:CD2	1:B:289:ILE:HD13	2.46	0.51
1:B:20:ASP:N	1:B:20:ASP:OD1	2.45	0.50
1:C:238:ILE:O	1:C:261:PHE:HB3	2.12	0.50
1:C:271:VAL:CG1	1:C:278:GLU:HG2	2.26	0.50
1:C:194:VAL:HA	4:C:452:GOL:H32	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:PHE:O	1:D:103:PHE:HD1	1.93	0.50
1:A:351:ARG:HG2	1:A:357:GLN:NE2	2.26	0.50
1:D:101:PHE:O	1:D:101:PHE:CD1	2.64	0.50
1:C:274:LEU:HD11	4:C:455:GOL:H12	1.94	0.50
1:C:236:ASP:HB3	1:C:259:GLN:HE21	1.76	0.49
1:C:333:GLN:OE1	1:C:380:ARG:HD3	2.12	0.49
1:C:69:ARG:NH1	1:D:104:SER:HA	2.28	0.49
1:D:333:GLN:OE1	1:D:380:ARG:HD3	2.12	0.49
1:B:35:ASP:OD1	1:B:305:ARG:NH1	2.45	0.49
1:D:238:ILE:O	1:D:261:PHE:HB3	2.13	0.49
1:C:320:ILE:N	1:C:320:ILE:HD12	2.28	0.49
1:A:150:VAL:CG1	1:A:151:ASN:N	2.76	0.49
1:D:203:PRO:HA	4:D:452:GOL:H11	1.95	0.49
1:D:125:ILE:HG22	1:D:153:PHE:O	2.12	0.49
1:D:286:LEU:C	1:D:286:LEU:HD12	2.32	0.49
1:D:211:PHE:CD2	1:D:289:ILE:HD13	2.48	0.48
1:D:36:THR:HG22	1:D:270:VAL:HG21	1.94	0.48
1:B:39:THR:CG2	1:B:269:SER:HB2	2.41	0.48
1:A:36:THR:HG22	1:A:270:VAL:HG21	1.94	0.48
1:B:283:HIS:HD2	1:B:300:PRO:HA	1.77	0.48
1:D:65:ASN:HB3	1:D:129:HIS:O	2.14	0.48
1:D:262:TYR:CD2	1:D:262:TYR:N	2.82	0.48
1:B:271:VAL:HG22	1:B:278:GLU:HG3	1.95	0.48
1:A:389:VAL:CG1	1:A:391:ASN:H	2.27	0.48
1:C:18:ALA:O	1:C:57:LEU:HA	2.13	0.48
1:B:80:ARG:O	1:B:84:MSE:HG3	2.13	0.48
1:B:351:ARG:HG2	1:B:357:GLN:NE2	2.28	0.48
1:D:87:ARG:HA	1:D:88:PRO:HD3	1.74	0.48
1:C:262:TYR:N	1:C:262:TYR:CD2	2.82	0.48
1:C:65:ASN:HB3	1:C:129:HIS:O	2.14	0.48
1:B:132:PRO:HA	1:B:138:LEU:O	2.14	0.47
1:A:39:THR:CG2	1:A:269:SER:HB2	2.43	0.47
1:B:175:LYS:HB3	1:B:210:TRP:CE3	2.48	0.47
1:D:251:ILE:HD11	1:D:285:GLY:N	2.29	0.47
1:D:284:VAL:CG1	1:D:285:GLY:N	2.77	0.47
1:D:80:ARG:O	1:D:84:MSE:HG3	2.14	0.47
1:A:250:LYS:CA	3:A:452:DTT:H11	2.43	0.47
1:B:325:ASN:O	1:B:328:VAL:HG12	2.15	0.47
1:C:389:VAL:CG1	1:C:391:ASN:H	2.27	0.47
1:B:262:TYR:CD2	1:B:262:TYR:N	2.82	0.47
1:D:284:VAL:HG12	1:D:285:GLY:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ASP:N	1:C:20:ASP:OD1	2.48	0.47
1:C:315:ALA:HB2	1:C:370:SER:O	2.15	0.47
1:D:101:PHE:CE1	1:D:148:GLY:O	2.68	0.47
1:D:93:ILE:HD12	1:D:99:VAL:CG1	2.45	0.47
1:B:265:GLN:HG2	1:B:265:GLN:O	2.15	0.47
1:C:87:ARG:HA	1:C:88:PRO:HD3	1.73	0.47
1:B:366:ARG:HG2	1:B:399:PHE:CE1	2.50	0.47
1:B:315:ALA:HB2	1:B:370:SER:O	2.15	0.47
1:D:37:PHE:CD1	1:D:74:THR:CG2	2.98	0.46
1:D:366:ARG:HG2	1:D:399:PHE:CE1	2.49	0.46
1:B:23:LEU:HD23	1:B:23:LEU:HA	1.79	0.46
1:D:39:THR:CG2	1:D:269:SER:HB2	2.44	0.46
1:A:132:PRO:HA	1:A:138:LEU:O	2.15	0.46
1:A:264:SER:OG	1:A:296:MSE:HE3	2.16	0.46
1:B:251:ILE:HD11	1:B:285:GLY:N	2.30	0.46
1:D:265:GLN:O	1:D:265:GLN:HG2	2.15	0.46
1:C:284:VAL:HG12	1:C:285:GLY:N	2.30	0.46
1:D:232:GLN:HG2	1:D:258:GLN:OE1	2.16	0.46
1:B:286:LEU:HD12	1:B:286:LEU:C	2.35	0.46
1:B:52:VAL:O	1:B:87:ARG:NH2	2.41	0.46
1:A:232:GLN:HG2	1:A:258:GLN:OE1	2.16	0.46
1:C:211:PHE:CD2	1:C:289:ILE:HD13	2.50	0.46
1:C:39:THR:CG2	1:C:269:SER:HB2	2.46	0.46
1:B:320:ILE:HD12	1:B:320:ILE:N	2.31	0.46
1:B:283:HIS:HD2	1:B:300:PRO:CA	2.28	0.46
1:D:320:ILE:HD12	1:D:320:ILE:N	2.31	0.46
1:B:65:ASN:HB3	1:B:129:HIS:O	2.16	0.46
1:A:122:VAL:HB	1:A:150:VAL:HG22	1.97	0.45
1:B:150:VAL:CG1	1:B:151:ASN:N	2.79	0.45
1:B:264:SER:OG	1:B:296:MSE:HE3	2.17	0.45
1:C:325:ASN:O	1:C:328:VAL:HG12	2.16	0.45
1:A:325:ASN:O	1:A:328:VAL:HG12	2.16	0.45
1:A:320:ILE:HD12	1:A:320:ILE:N	2.32	0.45
1:B:232:GLN:HG2	1:B:258:GLN:OE1	2.17	0.45
1:C:218:GLN:O	1:C:245:HIS:HB3	2.17	0.45
1:C:97:GLN:NE2	5:C:508:HOH:O	2.49	0.45
1:D:325:ASN:O	1:D:328:VAL:HG12	2.16	0.45
1:C:80:ARG:O	1:C:84:MSE:HG3	2.15	0.45
1:C:175:LYS:HB3	1:C:210:TRP:CE3	2.51	0.45
1:C:146:CYS:HA	4:C:454:GOL:H31	1.98	0.45
1:B:389:VAL:CG1	1:B:391:ASN:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:PHE:O	1:D:288:ARG:HA	2.16	0.45
1:C:284:VAL:CG1	1:C:285:GLY:N	2.80	0.45
1:D:315:ALA:HB2	1:D:370:SER:O	2.17	0.45
1:A:211:PHE:CD2	1:A:289:ILE:HD13	2.52	0.45
1:A:391:ASN:OD1	1:A:391:ASN:N	2.50	0.44
1:D:271:VAL:HG22	1:D:278:GLU:HG3	1.99	0.44
1:D:93:ILE:HD12	1:D:99:VAL:HG11	2.00	0.44
1:A:284:VAL:CG1	1:A:285:GLY:N	2.79	0.44
1:A:284:VAL:HG12	1:A:285:GLY:N	2.31	0.44
1:C:251:ILE:HD11	1:C:285:GLY:N	2.32	0.44
1:D:286:LEU:HD12	1:D:287:LEU:N	2.33	0.44
1:B:293:LYS:HA	5:B:512:HOH:O	2.17	0.44
1:C:13:PHE:O	1:C:288:ARG:HA	2.17	0.44
1:A:43:ILE:HG12	1:A:284:VAL:HG21	1.99	0.44
1:B:238:ILE:O	1:B:261:PHE:HB3	2.17	0.44
1:B:350:GLU:C	1:B:352:LEU:H	2.21	0.44
1:C:11:ASN:O	1:C:174:THR:HG23	2.17	0.44
1:B:391:ASN:OD1	1:B:391:ASN:N	2.50	0.44
1:A:175:LYS:HB3	1:A:210:TRP:CE3	2.53	0.44
1:B:13:PHE:CZ	1:B:171:LYS:HB2	2.53	0.44
1:C:174:THR:HB	1:C:291:GLY:H	1.83	0.43
1:B:251:ILE:HD11	1:B:285:GLY:CA	2.48	0.43
1:B:122:VAL:HB	1:B:150:VAL:HG22	2.00	0.43
1:D:175:LYS:HB3	1:D:210:TRP:CE3	2.53	0.43
1:D:391:ASN:ND2	1:D:394:ASP:O	2.50	0.43
1:C:259:GLN:O	1:C:260:LEU:HB2	2.18	0.43
1:C:138:LEU:HD22	1:D:138:LEU:HD22	2.00	0.43
1:D:250:LYS:HB2	1:D:265:GLN:HB3	2.00	0.43
1:C:286:LEU:C	1:C:286:LEU:HD12	2.38	0.43
1:D:251:ILE:HD11	1:D:285:GLY:CA	2.49	0.43
1:B:87:ARG:HA	1:B:88:PRO:HD3	1.74	0.43
1:C:352:LEU:HD12	1:C:352:LEU:HA	1.85	0.43
1:D:38:VAL:O	1:D:41:ASP:HB3	2.18	0.43
4:C:454:GOL:O1	5:C:508:HOH:O	2.21	0.43
1:D:391:ASN:N	1:D:391:ASN:OD1	2.52	0.43
1:C:327:LYS:HD2	1:C:327:LYS:HA	1.89	0.43
1:D:283:HIS:CD2	1:D:300:PRO:CA	3.00	0.43
1:B:38:VAL:O	1:B:41:ASP:HB3	2.18	0.43
1:A:229:ILE:HA	1:A:230:PRO:HD3	1.90	0.43
1:D:283:HIS:HD2	1:D:300:PRO:CA	2.31	0.43
1:C:38:VAL:O	1:C:41:ASP:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LEU:HD23	1:C:144:LEU:HA	1.73	0.43
1:B:391:ASN:ND2	1:B:394:ASP:O	2.52	0.43
1:C:391:ASN:N	1:C:391:ASN:OD1	2.52	0.43
1:A:13:PHE:O	1:A:288:ARG:HA	2.19	0.43
1:A:138:LEU:HD22	1:B:138:LEU:HD22	2.00	0.43
1:C:36:THR:HG22	1:C:270:VAL:HG21	2.00	0.43
1:A:327:LYS:HA	1:A:327:LYS:HD2	1.86	0.43
1:D:264:SER:OG	1:D:296:MSE:HE3	2.19	0.42
1:A:354:ASN:ND2	1:A:357:GLN:HG3	2.34	0.42
1:C:181:LEU:HA	1:C:181:LEU:HD12	1.78	0.42
1:D:100:ASN:ND2	1:D:103:PHE:HD2	2.18	0.42
1:C:229:ILE:HA	1:C:230:PRO:HD3	1.88	0.42
1:B:13:PHE:O	1:B:288:ARG:HA	2.19	0.42
1:D:101:PHE:C	1:D:103:PHE:H	2.22	0.42
1:B:229:ILE:HA	1:B:230:PRO:HD3	1.93	0.42
1:C:188:ARG:O	1:C:192:MSE:HG2	2.20	0.42
1:C:43:ILE:HG12	1:C:284:VAL:HG21	2.01	0.42
1:C:174:THR:HB	1:C:291:GLY:N	2.35	0.42
1:B:283:HIS:CD2	1:B:300:PRO:CA	2.99	0.42
1:A:350:GLU:C	1:A:352:LEU:H	2.21	0.42
1:D:259:GLN:O	1:D:260:LEU:HB2	2.19	0.42
1:D:81:LYS:HD3	1:D:82:TYR:CE1	2.55	0.42
1:A:65:ASN:HB3	1:A:129:HIS:O	2.19	0.42
1:B:43:ILE:HG12	1:B:284:VAL:HG21	2.01	0.42
1:C:366:ARG:HG2	1:C:399:PHE:CE1	2.53	0.42
1:C:200:MSE:CE	5:C:517:HOH:O	2.68	0.42
1:D:97:GLN:O	1:D:98:SER:HB2	2.20	0.42
1:C:136:ASP:CG	1:C:138:LEU:HG	2.40	0.42
1:B:383:GLN:HA	1:B:386:VAL:HG23	2.02	0.42
1:B:166:PRO:HG3	1:B:179:TYR:CZ	2.55	0.42
1:D:23:LEU:HD23	1:D:23:LEU:HA	1.80	0.42
1:D:143:ILE:O	1:D:146:CYS:HB3	2.20	0.42
1:A:315:ALA:HB2	1:A:370:SER:O	2.18	0.41
1:D:188:ARG:O	1:D:192:MSE:HG2	2.20	0.41
1:C:150:VAL:CG1	1:C:151:ASN:N	2.82	0.41
1:B:175:LYS:HB3	1:B:210:TRP:CZ3	2.56	0.41
1:C:52:VAL:O	1:C:87:ARG:NH2	2.45	0.41
1:C:26:MSE:HE1	4:C:455:GOL:H2	2.02	0.41
1:D:334:SER:O	1:D:338:GLU:HG2	2.21	0.41
1:A:15:ILE:HD13	1:A:54:PHE:CZ	2.56	0.41
1:C:21:ILE:HA	1:C:269:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ILE:H	1:C:320:ILE:HD12	1.86	0.41
1:C:196:LYS:HE2	4:C:452:GOL:O3	2.21	0.41
1:C:135:ALA:HB1	1:D:153:PHE:HA	2.03	0.41
4:C:454:GOL:O3	4:C:454:GOL:O1	2.34	0.41
1:C:262:TYR:CD2	1:C:294:MSE:CE	3.03	0.41
1:B:327:LYS:HD2	1:B:327:LYS:HA	1.86	0.41
1:A:139:CYS:O	1:A:140:ALA:C	2.58	0.41
1:D:389:VAL:HG11	1:D:395:ILE:HD12	2.03	0.41
1:D:181:LEU:HA	1:D:181:LEU:HD12	1.81	0.41
1:B:11:ASN:O	1:B:174:THR:HG23	2.19	0.41
1:A:366:ARG:HG2	1:A:399:PHE:CE1	2.50	0.41
1:C:251:ILE:HD11	1:C:285:GLY:CA	2.51	0.41
1:C:136:ASP:O	1:D:155:ARG:HD3	2.20	0.41
1:B:174:THR:HB	1:B:291:GLY:N	2.36	0.41
1:B:264:SER:CB	1:B:296:MSE:HE3	2.50	0.41
1:B:354:ASN:ND2	1:B:357:GLN:HG3	2.36	0.41
1:A:174:THR:HB	1:A:291:GLY:H	1.86	0.40
1:A:218:GLN:HG2	5:A:506:HOH:O	2.22	0.40
1:A:85:GLY:O	1:A:117:ASN:HB3	2.21	0.40
1:D:229:ILE:HA	1:D:230:PRO:HD3	1.90	0.40
1:A:136:ASP:CG	1:A:138:LEU:HG	2.42	0.40
1:D:43:ILE:HG12	1:D:284:VAL:HG21	2.03	0.40
1:C:250:LYS:HB2	1:C:265:GLN:HB3	2.04	0.40
1:C:252:ALA:HA	1:C:253:PRO:HD3	1.98	0.40
1:A:391:ASN:ND2	1:A:394:ASP:O	2.54	0.40
1:D:20:ASP:OD1	1:D:244:GLY:O	2.39	0.40
1:A:86:ASP:OD1	1:D:69:ARG:HG2	2.20	0.40
1:C:20:ASP:OD1	1:C:244:GLY:O	2.38	0.40
1:B:15:ILE:HD13	1:B:54:PHE:CZ	2.56	0.40
1:D:350:GLU:C	1:D:352:LEU:H	2.25	0.40
1:D:13:PHE:CZ	1:D:171:LYS:HB2	2.56	0.40
1:C:13:PHE:CZ	1:C:171:LYS:HB2	2.56	0.40
1:D:50:ASN:O	1:D:51:GLU:C	2.59	0.40
1:C:97:GLN:O	1:C:98:SER:HB2	2.21	0.40
1:A:129:HIS:CE1	4:A:454:GOL:H32	2.57	0.40
1:A:38:VAL:O	1:A:41:ASP:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/431 (86%)	347 (93%)	25 (7%)	0	100	100
1	B	374/431 (87%)	347 (93%)	25 (7%)	2 (0%)	34	76
1	C	373/431 (86%)	347 (93%)	24 (6%)	2 (0%)	34	76
1	D	382/431 (89%)	354 (93%)	25 (6%)	3 (1%)	24	66
All	All	1501/1724 (87%)	1395 (93%)	99 (7%)	7 (0%)	34	76

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	101	PHE
1	C	95	SER
1	D	104	SER
1	B	291	GLY
1	B	386	VAL
1	C	386	VAL
1	D	386	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	341/377 (90%)	307 (90%)	34 (10%)	9	34
1	B	343/377 (91%)	311 (91%)	32 (9%)	11	39
1	C	342/377 (91%)	307 (90%)	35 (10%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	350/377 (93%)	315 (90%)	35 (10%)	9	34
All	All	1376/1508 (91%)	1240 (90%)	136 (10%)	10	35

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	20	ASP
1	A	64	GLU
1	A	72	LEU
1	A	96	ASP
1	A	97	GLN
1	A	174	THR
1	A	188	ARG
1	A	192	MSE
1	A	199	THR
1	A	202	ARG
1	A	232	GLN
1	A	235	ASP
1	A	254	THR
1	A	255	LYS
1	A	259	GLN
1	A	261	PHE
1	A	262	TYR
1	A	270	VAL
1	A	286	LEU
1	A	294	MSE
1	A	319	ASP
1	A	324	ASP
1	A	327	LYS
1	A	330	GLN
1	A	345	GLU
1	A	355	SER
1	A	364	ARG
1	A	365	LEU
1	A	366	ARG
1	A	369	TYR
1	A	389	VAL
1	A	396	ILE
1	A	400	ARG
1	B	9	ASP
1	B	20	ASP

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Mol	Chain	Res	Type
1	B	52	VAL
1	B	64	GLU
1	B	72	LEU
1	B	174	THR
1	B	188	ARG
1	B	192	MSE
1	B	199	THR
1	B	202	ARG
1	B	232	GLN
1	B	235	ASP
1	B	254	THR
1	B	255	LYS
1	B	259	GLN
1	B	262	TYR
1	B	270	VAL
1	B	286	LEU
1	B	294	MSE
1	B	319	ASP
1	B	324	ASP
1	B	327	LYS
1	B	330	GLN
1	B	345	GLU
1	B	355	SER
1	B	364	ARG
1	B	365	LEU
1	B	366	ARG
1	B	369	TYR
1	B	389	VAL
1	B	396	ILE
1	B	400	ARG
1	C	9	ASP
1	C	19	THR
1	C	20	ASP
1	C	52	VAL
1	C	64	GLU
1	C	72	LEU
1	C	96	ASP
1	C	98	SER
1	C	115	ASN
1	C	174	THR
1	C	188	ARG
1	C	192	MSE

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Mol	Chain	Res	Type
1	C	199	THR
1	C	202	ARG
1	C	232	GLN
1	C	235	ASP
1	C	254	THR
1	C	255	LYS
1	C	259	GLN
1	C	262	TYR
1	C	270	VAL
1	C	286	LEU
1	C	294	MSE
1	C	319	ASP
1	C	324	ASP
1	C	327	LYS
1	C	330	GLN
1	C	345	GLU
1	C	355	SER
1	C	364	ARG
1	C	365	LEU
1	C	366	ARG
1	C	389	VAL
1	C	396	ILE
1	C	400	ARG
1	D	9	ASP
1	D	20	ASP
1	D	64	GLU
1	D	72	LEU
1	D	96	ASP
1	D	101	PHE
1	D	103	PHE
1	D	104	SER
1	D	105	LYS
1	D	174	THR
1	D	188	ARG
1	D	192	MSE
1	D	199	THR
1	D	202	ARG
1	D	232	GLN
1	D	235	ASP
1	D	254	THR
1	D	255	LYS
1	D	259	GLN

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Mol	Chain	Res	Type
1	D	262	TYR
1	D	270	VAL
1	D	286	LEU
1	D	294	MSE
1	D	319	ASP
1	D	324	ASP
1	D	327	LYS
1	D	330	GLN
1	D	345	GLU
1	D	355	SER
1	D	364	ARG
1	D	365	LEU
1	D	366	ARG
1	D	389	VAL
1	D	396	ILE
1	D	400	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	218	GLN
1	A	357	GLN
1	B	283	HIS
1	B	357	GLN
1	C	218	GLN
1	C	283	HIS
1	C	357	GLN
1	D	129	HIS
1	D	283	HIS
1	D	357	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 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	DTT	A	451	-	7,7,7	0.80	0	4,8,8	1.01	0
3	DTT	A	452	-	7,7,7	0.92	0	4,8,8	2.38	1 (25%)
4	GOL	A	453	-	5,5,5	0.34	0	5,5,5	0.32	0
4	GOL	A	454	-	5,5,5	0.28	0	5,5,5	0.41	0
4	GOL	A	455	-	5,5,5	0.31	0	5,5,5	0.17	0
4	GOL	A	456	-	5,5,5	0.35	0	5,5,5	0.35	0
4	GOL	A	457	-	5,5,5	0.30	0	5,5,5	0.40	0
4	GOL	A	458	-	5,5,5	0.35	0	5,5,5	0.47	0
4	GOL	C	451	-	5,5,5	0.31	0	5,5,5	0.50	0
4	GOL	C	452	-	5,5,5	0.33	0	5,5,5	0.24	0
4	GOL	C	453	-	5,5,5	0.38	0	5,5,5	0.42	0
4	GOL	C	454	-	5,5,5	0.28	0	5,5,5	0.39	0
4	GOL	C	455	-	5,5,5	0.30	0	5,5,5	0.43	0
4	GOL	C	456	-	5,5,5	0.38	0	5,5,5	0.29	0
4	GOL	D	451	-	5,5,5	0.34	0	5,5,5	0.39	0
4	GOL	D	452	-	5,5,5	0.35	0	5,5,5	0.84	0
4	GOL	D	453	-	5,5,5	0.32	0	5,5,5	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTT	A	451	-	-	0/8/8/8	0/0/0/0
3	DTT	A	452	-	-	0/8/8/8	0/0/0/0
4	GOL	A	453	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	454	-	-	0/4/4/4	0/0/0/0
4	GOL	A	455	-	-	0/4/4/4	0/0/0/0
4	GOL	A	456	-	-	0/4/4/4	0/0/0/0
4	GOL	A	457	-	-	0/4/4/4	0/0/0/0
4	GOL	A	458	-	-	0/4/4/4	0/0/0/0
4	GOL	C	451	-	-	0/4/4/4	0/0/0/0
4	GOL	C	452	-	-	0/4/4/4	0/0/0/0
4	GOL	C	453	-	-	0/4/4/4	0/0/0/0
4	GOL	C	454	-	-	0/4/4/4	0/0/0/0
4	GOL	C	455	-	-	0/4/4/4	0/0/0/0
4	GOL	C	456	-	-	0/4/4/4	0/0/0/0
4	GOL	D	451	-	-	0/4/4/4	0/0/0/0
4	GOL	D	452	-	-	0/4/4/4	0/0/0/0
4	GOL	D	453	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	452	DTT	C2-C1-S1	4.54	121.44	113.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	452	DTT	4	0
4	A	454	GOL	1	0
4	C	452	GOL	2	0
4	C	453	GOL	1	0
4	C	454	GOL	3	0
4	C	455	GOL	2	0
4	C	456	GOL	2	0
4	D	452	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	367/431 (85%)	0.00	14 (3%) 44 18	39, 68, 165, 187	0
1	B	369/431 (85%)	0.29	39 (10%) 8 3	42, 70, 168, 188	0
1	C	368/431 (85%)	0.01	12 (3%) 50 22	40, 67, 166, 187	1 (0%)
1	D	377/431 (87%)	0.34	51 (13%) 4 1	39, 71, 168, 190	1 (0%)
All	All	1481/1724 (85%)	0.16	116 (7%) 16 6	39, 69, 167, 190	2 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	225	SER	8.3
1	D	370	SER	6.9
1	D	323	PRO	6.7
1	B	316	ASN	6.1
1	D	322	ASN	5.9
1	D	376	PHE	5.9
1	B	313	VAL	5.4
1	B	321	PHE	5.3
1	D	371	GLY	5.3
1	A	372	GLY	5.3
1	D	332	ILE	4.9
1	B	372	GLY	4.7
1	D	313	VAL	4.6
1	D	398	PHE	4.5
1	D	378	VAL	4.5
1	B	371	GLY	4.5
1	D	336	CYS	4.5
1	D	381	PHE	4.5
1	B	318	PRO	4.3
1	B	315	ALA	4.2
1	D	316	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	375	PRO	4.2
1	B	376	PHE	4.1
1	D	328	VAL	4.1
1	C	315	ALA	4.1
1	B	324	ASP	4.0
1	B	317	HIS	4.0
1	B	373	PHE	4.0
1	A	226	THR	3.9
1	D	315	ALA	3.8
1	B	375	PRO	3.7
1	A	312	ILE	3.7
1	C	321	PHE	3.7
1	A	327	LYS	3.7
1	D	373	PHE	3.6
1	B	332	ILE	3.6
1	B	328	VAL	3.6
1	B	226	THR	3.5
1	B	374	GLU	3.4
1	D	319	ASP	3.4
1	D	374	GLU	3.4
1	D	340	ILE	3.3
1	D	329	THR	3.3
1	B	385	PHE	3.3
1	B	362	LEU	3.2
1	B	323	PRO	3.2
1	B	320	ILE	3.2
1	D	226	THR	3.1
1	B	336	CYS	3.1
1	B	370	SER	3.1
1	D	382	SER	3.1
1	D	385	PHE	3.1
1	A	373	PHE	3.1
1	B	398	PHE	3.1
1	C	326	PRO	3.1
1	B	377	SER	3.0
1	A	314	LEU	3.0
1	B	329	THR	3.0
1	D	311	ASP	2.9
1	B	314	LEU	2.9
1	D	321	PHE	2.8
1	B	331	ALA	2.8
1	B	383	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	371	GLY	2.7
1	A	374	GLU	2.7
1	D	333	GLN	2.7
1	D	312	ILE	2.7
1	C	318	PRO	2.7
1	D	160	GLU	2.6
1	B	311	ASP	2.6
1	D	107	PRO	2.6
1	C	329	THR	2.6
1	D	380	ARG	2.6
1	A	331	ALA	2.6
1	D	310	GLU	2.6
1	B	381	PHE	2.5
1	B	368	ASP	2.5
1	C	314	LEU	2.5
1	A	320	ILE	2.5
1	D	317	HIS	2.5
1	D	368	ASP	2.5
1	A	326	PRO	2.4
1	D	314	LEU	2.4
1	C	330	GLN	2.4
1	C	312	ILE	2.3
1	D	399	PHE	2.3
1	D	324	ASP	2.3
1	D	366	ARG	2.3
1	C	375	PRO	2.3
1	B	312	ILE	2.3
1	D	369	TYR	2.3
1	D	308	PHE	2.3
1	C	226	THR	2.3
1	D	318	PRO	2.3
1	D	326	PRO	2.3
1	B	365	LEU	2.3
1	D	335	PHE	2.3
1	C	371	GLY	2.2
1	D	327	LYS	2.2
1	C	115	ASN	2.2
1	B	327	LYS	2.2
1	A	370	SER	2.2
1	D	365	LEU	2.2
1	A	400	ARG	2.2
1	D	367	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	335	PHE	2.1
1	D	338	GLU	2.1
1	B	378	VAL	2.1
1	D	320	ILE	2.1
1	B	352	LEU	2.1
1	D	339	LYS	2.1
1	D	372	GLY	2.1
1	B	319	ASP	2.1
1	D	104	SER	2.0
1	B	393	LYS	2.0
1	A	381	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
4	GOL	C	453	6/6	0.80	0.38	5.71	69,91,92,98	0
4	GOL	C	454	6/6	0.90	0.42	5.67	78,81,86,93	0
4	GOL	D	452	6/6	0.82	0.50	4.41	76,90,106,106	0
4	GOL	C	455	6/6	0.95	0.38	3.77	70,87,99,106	0
4	GOL	D	453	6/6	0.78	0.38	3.52	71,88,104,109	0
3	DTT	A	452	8/8	0.80	0.30	3.28	82,96,109,110	0
4	GOL	C	456	6/6	0.88	0.34	2.64	72,81,92,98	0
4	GOL	A	458	6/6	0.74	0.28	2.08	82,101,108,109	0
2	MN	B	412	1/1	0.97	0.21	1.97	56,56,56,56	0
4	GOL	A	455	6/6	0.92	0.24	1.38	66,84,89,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MN	A	412	1/1	0.98	0.19	0.96	46,46,46,46	0
2	MN	D	412	1/1	0.98	0.19	0.71	58,58,58,58	0
2	MN	A	413	1/1	0.53	0.18	0.29	107,107,107,107	0
2	MN	C	412	1/1	0.99	0.19	0.24	42,42,42,42	0
4	GOL	C	451	6/6	0.87	0.21	-0.09	78,86,89,93	0
2	MN	B	413	1/1	0.74	0.12	-1.60	99,99,99,99	0
2	MN	D	413	1/1	0.92	0.12	-3.09	111,111,111,111	0
2	MN	C	413	1/1	0.75	0.10	-6.01	99,99,99,99	0
4	GOL	C	452	6/6	0.89	0.36	-	74,85,92,105	0
4	GOL	A	456	6/6	0.90	0.23	-	77,85,95,100	0
4	GOL	A	454	6/6	0.90	0.21	-	55,75,88,95	0
3	DTT	A	451	8/8	0.74	0.34	-	98,127,143,146	0
4	GOL	A	453	6/6	0.87	0.30	-	84,92,97,103	0
4	GOL	D	451	6/6	0.85	0.27	-	68,85,100,102	0
4	GOL	A	457	6/6	0.89	0.24	-	89,95,114,119	0

6.5 Other polymers

There are no such residues in this entry.