



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:17 AM GMT

PDB ID : 3VYL
Title : Structure of L-ribulose 3-epimerase
Authors : Uechi, K.; Sakuraba, H.; Takata, G.
Deposited on : 2012-09-27
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

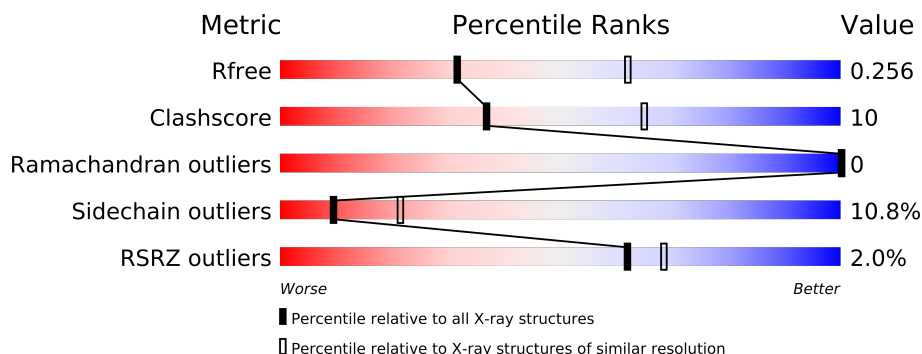
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. 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	297	
1	B	297	
1	C	297	
1	D	297	
1	E	297	
1	F	297	
1	G	297	
1	H	297	

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	MPD	A	1002	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	MPD	B	1002	-	X
3	MPD	D	1002	-	X
3	MPD	E	1002	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18302 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 L-ribulose 3-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	B	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	C	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	D	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	E	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	F	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	G	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	H	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			

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

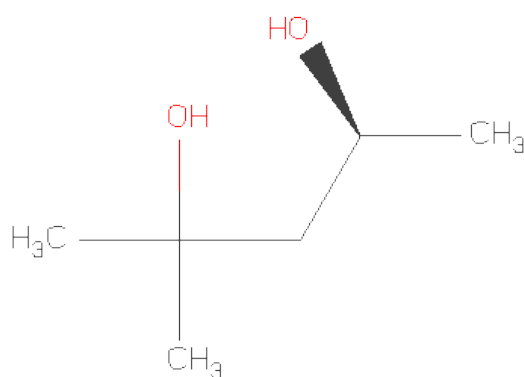
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	H	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	60	Total	O	0	0
			60	60		
4	C	64	Total	O	0	0
			64	64		

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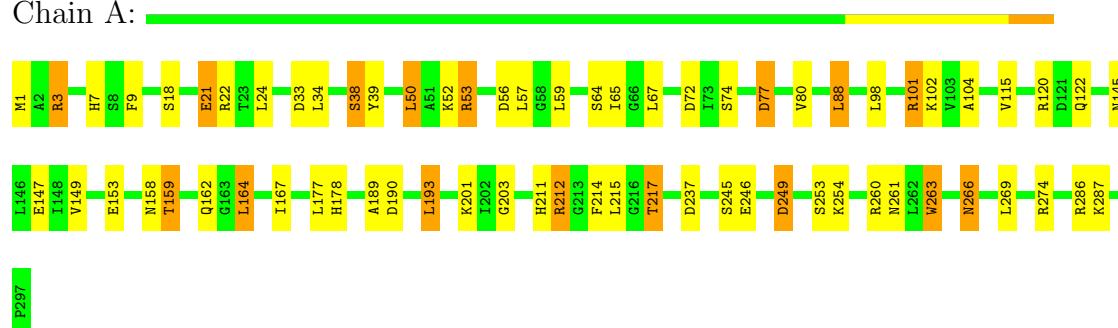
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	72	Total 72	O 72	0	0
4	E	29	Total 29	O 29	0	0
4	F	11	Total 11	O 11	0	0
4	G	11	Total 11	O 11	0	0
4	H	21	Total 21	O 21	0	0

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.

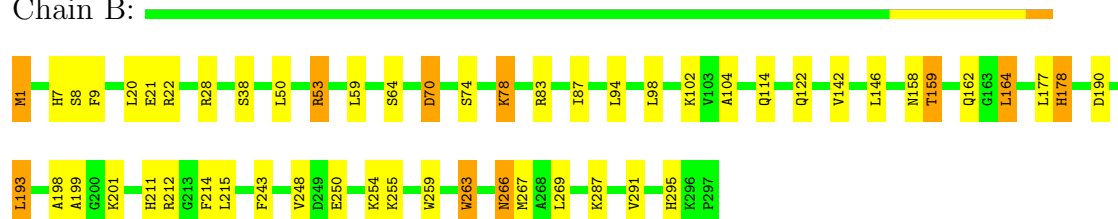
- Molecule 1: L-ribulose 3-epimerase

Chain A:



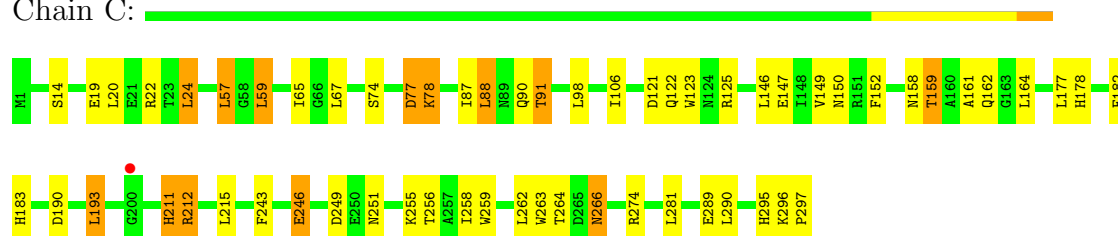
- Molecule 1: L-ribulose 3-epimerase

Chain B:



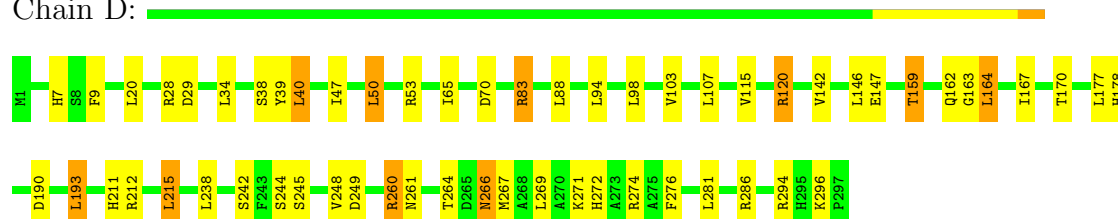
- Molecule 1: L-ribulose 3-epimerase

Chain C:



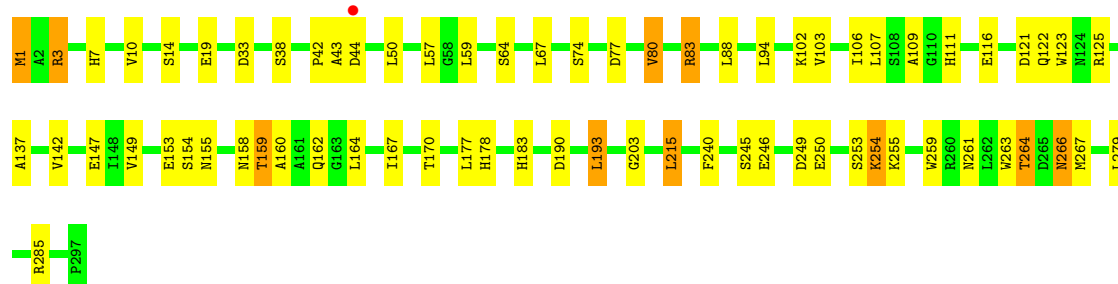
- Molecule 1: L-ribulose 3-epimerase

Chain D:



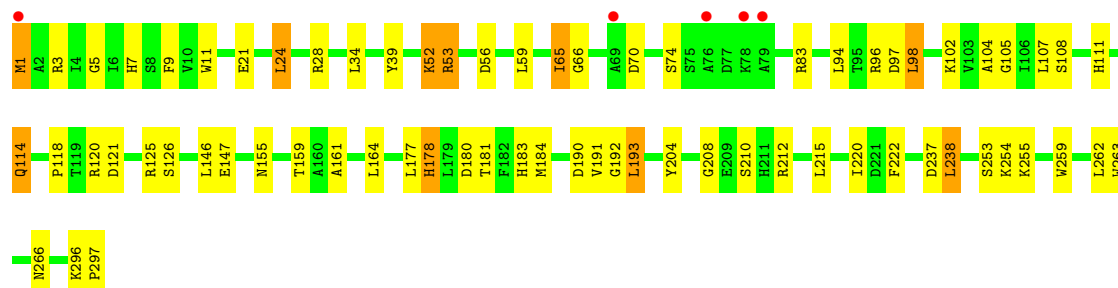
- Molecule 1: L-ribulose 3-epimerase

Chain E:



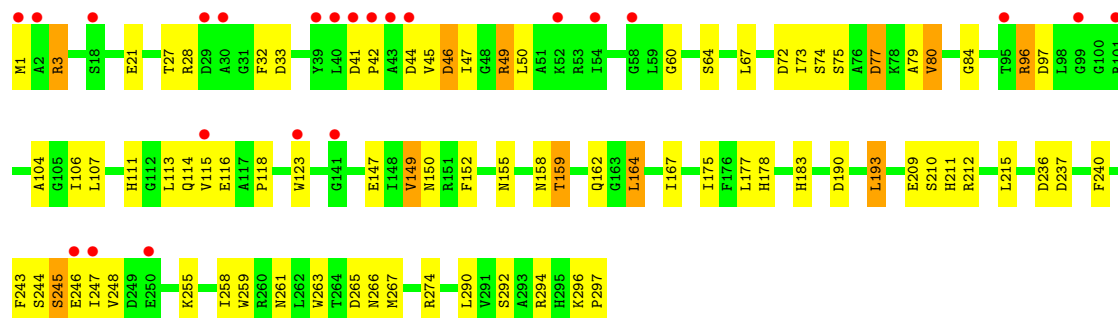
- Molecule 1: L-ribulose 3-epimerase

Chain F:



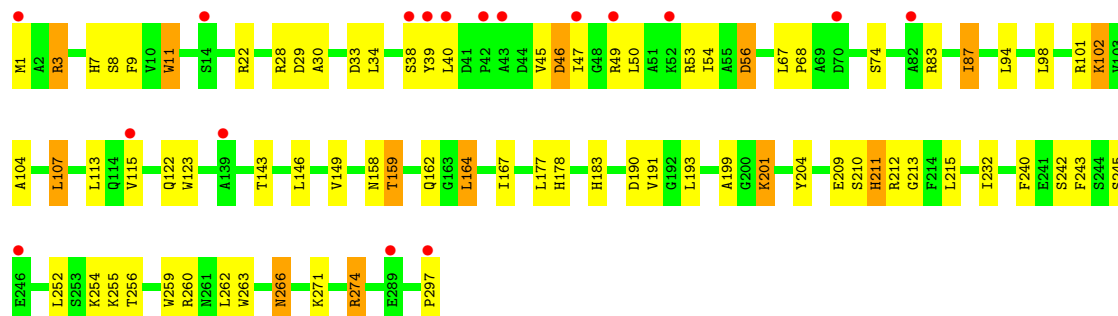
- Molecule 1: L-ribulose 3-epimerase

Chain G:



- Molecule 1: L-ribulose 3-epimerase

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	202.51Å 206.23Å 121.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.48 – 2.70 34.48 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.48-2.70) 99.6 (34.48-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.16 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.264 0.202 , 0.256	Depositor DCC
R_{free} test set	3536 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 23.0	EDS
Estimated twinning fraction	0.004 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 70175 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18302	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: MPD, MN

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	0.67	2/2278 (0.1%)	0.66	0/3082
1	B	0.68	2/2278 (0.1%)	0.66	0/3082
1	C	0.66	1/2278 (0.0%)	0.67	0/3082
1	D	0.72	0/2278	0.65	0/3082
1	E	0.69	1/2278 (0.0%)	0.64	0/3082
1	F	0.65	3/2278 (0.1%)	0.65	0/3082
1	G	0.68	2/2278 (0.1%)	0.67	0/3082
1	H	0.67	2/2278 (0.1%)	0.64	1/3082 (0.0%)
All	All	0.68	13/18224 (0.1%)	0.66	1/24656 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	259	TRP	CD2-CE2	5.42	1.47	1.41
1	F	259	TRP	CD2-CE2	5.40	1.47	1.41
1	A	263	TRP	CD2-CE2	5.37	1.47	1.41
1	H	123	TRP	CD2-CE2	5.32	1.47	1.41
1	A	153	GLU	CD-OE1	-5.31	1.19	1.25
1	G	263	TRP	CD2-CE2	5.28	1.47	1.41
1	B	263	TRP	CD2-CE2	5.27	1.47	1.41
1	H	259	TRP	CD2-CE2	5.26	1.47	1.41
1	F	11	TRP	CD2-CE2	5.22	1.47	1.41
1	F	263	TRP	CD2-CE2	5.21	1.47	1.41
1	C	123	TRP	CD2-CE2	5.08	1.47	1.41
1	G	123	TRP	CD2-CE2	5.06	1.47	1.41
1	B	259	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	11	TRP	N-CA-C	5.38	125.53	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	2242	0	2229	64	0
1	B	2242	0	2229	32	0
1	C	2242	0	2229	44	0
1	D	2242	0	2229	34	0
1	E	2242	0	2229	48	0
1	F	2242	0	2229	50	0
1	G	2242	0	2229	63	0
1	H	2242	0	2229	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	8	0	14	0	0
3	B	8	0	14	1	0
3	D	8	0	14	1	0
3	E	8	0	14	1	0
4	A	58	0	0	0	0
4	B	60	0	0	1	0
4	C	64	0	0	1	0
4	D	72	0	0	0	0
4	E	29	0	0	1	0
4	F	11	0	0	0	0
4	G	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	21	0	0	0	0
All	All	18302	0	17888	367	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 10.

All (367) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:78:LYS:CD	1:C:78:LYS:H	1.50	1.18
1:G:3:ARG:HH21	1:G:60:GLY:CA	1.56	1.17
1:C:78:LYS:N	1:C:78:LYS:HD2	1.51	1.15
1:D:39:TYR:O	1:D:40:LEU:HD13	1.48	1.10
1:F:53:ARG:HG3	1:F:53:ARG:HH11	1.00	1.09
1:E:1:MET:O	1:E:1:MET:HG2	1.54	1.05
1:A:101:ARG:HH11	1:A:101:ARG:HG3	1.21	1.04
1:B:78:LYS:HE3	1:B:78:LYS:H	1.22	1.03
1:G:45:VAL:HG12	1:G:46:ASP:H	1.22	1.01
1:G:3:ARG:NH2	1:G:60:GLY:CA	2.24	1.00
1:H:211:HIS:O	1:H:212:ARG:HB2	1.61	0.99
1:H:190:ASP:HB3	1:H:193:LEU:HB2	1.45	0.97
1:H:159:THR:HG22	1:H:162:GLN:H	1.30	0.95
1:G:149:VAL:HG12	1:G:183:HIS:CD2	2.01	0.95
1:A:1:MET:HG2	1:A:1:MET:O	1.66	0.94
1:E:102:LYS:HE2	1:E:203:GLY:O	1.67	0.94
1:C:78:LYS:HD2	1:C:78:LYS:H	0.77	0.94
1:A:212:ARG:CG	1:A:212:ARG:HH11	1.80	0.93
1:F:53:ARG:HG3	1:F:53:ARG:NH1	1.79	0.93
1:G:45:VAL:CG1	1:G:46:ASP:H	1.82	0.93
1:A:53:ARG:HH11	1:A:53:ARG:HG3	1.34	0.93
1:D:7:HIS:HD2	1:D:9:PHE:H	1.18	0.92
1:C:212:ARG:HG3	4:C:1113:HOH:O	1.69	0.91
1:G:45:VAL:HG12	1:G:46:ASP:N	1.81	0.91
1:G:3:ARG:HH21	1:G:60:GLY:HA2	1.32	0.90
1:H:242:SER:O	1:H:243:PHE:HD1	1.53	0.89
4:B:1106:HOH:O	1:D:159:THR:HG21	1.73	0.88
1:D:190:ASP:HB3	1:D:193:LEU:HB2	1.55	0.88
1:F:238:LEU:O	1:F:238:LEU:HD12	1.74	0.88
1:B:159:THR:HG22	1:B:162:GLN:H	1.39	0.88
1:G:3:ARG:HH21	1:G:60:GLY:HA3	1.38	0.87
1:H:7:HIS:HD2	1:H:9:PHE:H	1.21	0.86
1:D:120:ARG:HG3	1:D:120:ARG:HH21	1.40	0.86
1:A:212:ARG:HG2	1:A:212:ARG:HH11	1.42	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:286:ARG:HG2	1:D:286:ARG:HH11	1.42	0.84
1:H:242:SER:O	1:H:243:PHE:CD1	2.30	0.84
1:F:190:ASP:HB3	1:F:193:LEU:HB2	1.60	0.84
1:C:87:ILE:O	1:C:91:THR:HG23	1.80	0.81
1:A:3:ARG:HD2	1:A:33:ASP:OD1	1.80	0.81
1:A:211:HIS:CE1	1:A:217:THR:HG22	2.16	0.80
1:F:238:LEU:O	1:F:238:LEU:CD1	2.30	0.80
1:D:39:TYR:O	1:D:40:LEU:CD1	2.29	0.80
1:E:1:MET:CG	1:E:1:MET:O	2.30	0.80
1:E:3:ARG:HG2	1:E:3:ARG:HH11	1.46	0.80
1:A:266:ASN:H	1:A:266:ASN:HD22	1.27	0.79
1:D:164:LEU:HD13	1:D:177:LEU:HD11	1.65	0.79
1:H:211:HIS:HD2	1:H:213:GLY:H	1.29	0.78
1:G:190:ASP:HB3	1:G:193:LEU:HB2	1.65	0.78
1:B:266:ASN:H	1:B:266:ASN:HD22	1.32	0.77
1:A:53:ARG:NH1	1:A:53:ARG:HG3	1.95	0.77
1:F:111:HIS:O	1:F:255:LYS:HE3	1.85	0.77
1:A:159:THR:HG22	1:A:162:GLN:H	1.49	0.76
1:E:279:LEU:HD23	3:E:1002:MPD:HM2	1.67	0.76
1:F:7:HIS:HD2	1:F:9:PHE:H	1.33	0.76
1:C:190:ASP:HB3	1:C:193:LEU:HB2	1.67	0.76
1:G:243:PHE:HB3	1:G:248:VAL:HG21	1.68	0.76
1:E:159:THR:HG22	1:E:162:GLN:H	1.50	0.76
1:G:64:SER:HA	1:G:104:ALA:O	1.85	0.76
1:A:266:ASN:HD22	1:A:266:ASN:N	1.86	0.73
1:A:190:ASP:HB3	1:A:193:LEU:HB2	1.69	0.73
1:E:3:ARG:HB3	1:E:33:ASP:HB2	1.69	0.73
1:E:83:ARG:HH11	1:E:83:ARG:CG	2.02	0.73
1:C:159:THR:HG22	1:C:162:GLN:H	1.53	0.73
1:F:120:ARG:HG3	1:H:297:PRO:O	1.89	0.72
1:A:145:ASN:HD22	1:A:203:GLY:HA3	1.54	0.71
1:F:238:LEU:H	1:F:238:LEU:HD12	1.55	0.71
1:G:111:HIS:O	1:G:255:LYS:NZ	2.24	0.71
1:F:159:THR:HG22	1:F:161:ALA:H	1.54	0.71
1:A:77:ASP:CG	1:A:80:VAL:HG23	2.11	0.70
1:B:266:ASN:N	1:B:266:ASN:HD22	1.88	0.70
1:H:3:ARG:HB3	1:H:33:ASP:HB2	1.74	0.70
1:C:77:ASP:OD1	1:C:77:ASP:C	2.29	0.70
1:A:101:ARG:HH12	1:A:102:LYS:HE2	1.57	0.69
1:G:77:ASP:C	1:G:77:ASP:OD1	2.29	0.69
1:G:3:ARG:NH2	1:G:60:GLY:N	2.39	0.69
1:G:150:ASN:OD1	1:G:150:ASN:C	2.30	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:209:GLU:HG3	1:H:210:SER:N	2.07	0.69
1:D:159:THR:HG22	1:D:162:GLN:H	1.58	0.69
4:E:1123:HOH:O	1:G:159:THR:HG21	1.92	0.68
1:A:77:ASP:OD1	1:A:77:ASP:C	2.30	0.68
1:B:70:ASP:OD1	1:B:70:ASP:C	2.30	0.68
1:H:164:LEU:HD13	1:H:177:LEU:HD11	1.76	0.67
1:H:74:SER:HB3	1:H:122:GLN:HG3	1.75	0.67
1:G:77:ASP:OD1	1:G:80:VAL:HG22	1.95	0.67
1:C:14:SER:HB3	1:C:19:GLU:HG2	1.77	0.67
1:A:246:GLU:OE2	1:A:246:GLU:HA	1.94	0.66
1:A:145:ASN:ND2	1:A:203:GLY:HA3	2.10	0.66
1:G:77:ASP:O	1:G:80:VAL:HG23	1.95	0.66
1:G:106:ILE:HD12	1:G:111:HIS:CD2	2.31	0.66
1:G:3:ARG:HB3	1:G:237:ASP:OD1	1.97	0.65
1:G:67:LEU:CD1	1:G:73:ILE:HG23	2.26	0.65
1:A:263:TRP:CZ3	1:A:266:ASN:HB3	2.31	0.65
1:G:67:LEU:HD13	1:G:73:ILE:HG23	1.78	0.65
1:H:46:ASP:OD2	1:H:46:ASP:N	2.29	0.65
1:B:7:HIS:HD2	1:B:9:PHE:H	1.45	0.65
1:F:114:GLN:HE21	1:F:114:GLN:HA	1.61	0.64
1:G:77:ASP:OD1	1:G:79:ALA:N	2.29	0.64
1:B:263:TRP:CZ3	1:B:266:ASN:HB3	2.33	0.64
1:A:212:ARG:HG2	1:A:212:ARG:NH1	2.13	0.64
1:A:38:SER:O	1:A:65:ILE:HG22	1.98	0.64
1:A:7:HIS:HD2	1:A:9:PHE:H	1.44	0.64
1:A:266:ASN:ND2	1:A:266:ASN:H	1.95	0.63
1:A:245:SER:HB3	1:A:261:ASN:HD21	1.63	0.63
1:A:101:ARG:NH1	1:A:101:ARG:HG3	1.98	0.63
1:E:14:SER:HB3	1:E:19:GLU:HG2	1.80	0.63
1:F:181:THR:HG21	1:F:222:PHE:HE2	1.64	0.63
1:H:211:HIS:CD2	1:H:213:GLY:H	2.14	0.62
1:G:42:PRO:HB3	1:G:47:ILE:HD11	1.81	0.62
1:A:211:HIS:HE1	1:A:217:THR:HG22	1.60	0.62
1:F:181:THR:HG21	1:F:222:PHE:CE2	2.34	0.62
1:E:77:ASP:HB3	1:E:80:VAL:HG13	1.82	0.61
1:B:190:ASP:HB3	1:B:193:LEU:HB2	1.81	0.61
1:A:212:ARG:HG3	1:A:212:ARG:HH11	1.64	0.61
1:F:53:ARG:CG	1:F:53:ARG:HH11	1.91	0.61
1:D:120:ARG:HG3	1:D:120:ARG:NH2	2.10	0.61
1:D:245:SER:HB2	1:D:261:ASN:HD21	1.66	0.61
1:H:53:ARG:HA	1:H:56:ASP:HB2	1.80	0.61
1:B:50:LEU:HD23	1:B:98:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:236:ASP:OD1	1:G:237:ASP:N	2.30	0.60
1:F:147:GLU:HA	1:F:178:HIS:O	2.01	0.60
1:H:242:SER:C	1:H:243:PHE:CD1	2.75	0.60
1:G:77:ASP:O	1:G:80:VAL:CG2	2.50	0.60
1:E:154:SER:OG	1:E:155:ASN:N	2.31	0.60
1:C:266:ASN:HD22	1:C:266:ASN:N	2.00	0.60
1:F:238:LEU:CD1	1:F:238:LEU:C	2.70	0.60
1:C:78:LYS:N	1:C:78:LYS:CD	2.30	0.59
1:B:266:ASN:ND2	1:B:266:ASN:H	2.00	0.59
1:F:114:GLN:HG2	1:F:155:ASN:ND2	2.17	0.59
1:B:1:MET:SD	3:B:1002:MPD:H12	2.42	0.59
1:A:164:LEU:HD13	1:A:177:LEU:HD11	1.84	0.59
1:A:53:ARG:HH11	1:A:53:ARG:CG	2.09	0.59
1:B:164:LEU:HD13	1:B:177:LEU:HD11	1.85	0.59
1:A:9:PHE:CZ	1:A:38:SER:HB3	2.37	0.58
1:B:78:LYS:CE	1:B:78:LYS:H	2.07	0.58
1:G:3:ARG:NH2	1:G:60:GLY:HA2	2.01	0.58
1:E:3:ARG:NH1	1:E:3:ARG:HG2	2.16	0.58
1:G:64:SER:CA	1:G:104:ALA:O	2.52	0.58
1:F:7:HIS:CD2	1:F:9:PHE:H	2.17	0.58
1:D:47:ILE:HG23	1:D:98:LEU:HD13	1.86	0.58
1:A:249:ASP:OD2	1:A:249:ASP:C	2.42	0.57
1:D:163:GLY:O	1:D:167:ILE:HG13	2.05	0.57
1:E:7:HIS:O	1:E:10:VAL:HG13	2.04	0.57
1:H:50:LEU:O	1:H:54:ILE:HG12	2.05	0.57
1:A:120:ARG:HH11	1:C:296:LYS:HD2	1.70	0.57
1:D:286:ARG:HG2	1:D:286:ARG:NH1	2.09	0.57
1:C:74:SER:HB2	1:C:122:GLN:HG3	1.86	0.57
1:B:83:ARG:O	1:B:87:ILE:HG13	2.04	0.56
1:C:266:ASN:ND2	1:C:266:ASN:H	2.04	0.56
1:F:94:LEU:HG	1:F:98:LEU:HD22	1.87	0.56
1:A:167:ILE:HG21	1:A:201:LYS:HE3	1.86	0.56
1:E:83:ARG:HH11	1:E:83:ARG:HG3	1.70	0.56
1:H:7:HIS:CD2	1:H:9:PHE:H	2.13	0.56
1:B:162:GLN:HB3	1:D:294:ARG:O	2.05	0.56
1:E:38:SER:HA	1:E:64:SER:O	2.05	0.56
1:E:147:GLU:HA	1:E:178:HIS:O	2.06	0.55
1:E:121:ASP:O	1:E:125:ARG:HB2	2.05	0.55
1:C:24:LEU:HB3	1:C:57:LEU:HD23	1.88	0.55
1:H:209:GLU:HG3	1:H:210:SER:H	1.70	0.55
1:E:250:GLU:HG2	1:E:254:LYS:NZ	2.21	0.55
1:A:189:ALA:HB2	1:C:290:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:111:HIS:NE2	1:E:153:GLU:OE2	2.27	0.55
1:E:266:ASN:HD22	1:E:267:MET:N	2.05	0.55
1:A:1:MET:CG	1:A:1:MET:O	2.46	0.55
1:D:266:ASN:HD22	1:D:267:MET:N	2.04	0.54
1:E:190:ASP:HB3	1:E:193:LEU:HB2	1.89	0.54
1:G:77:ASP:CG	1:G:80:VAL:HG22	2.27	0.54
1:G:164:LEU:HD13	1:G:177:LEU:HD11	1.88	0.54
1:G:45:VAL:CG1	1:G:46:ASP:N	2.46	0.54
1:G:159:THR:HG22	1:G:162:GLN:H	1.72	0.54
1:F:3:ARG:HB3	1:F:237:ASP:OD1	2.08	0.53
1:A:149:VAL:O	1:A:158:ASN:HA	2.09	0.53
1:F:96:ARG:NH1	1:F:97:ASP:OD1	2.40	0.53
1:D:103:VAL:HG23	1:D:142:VAL:HG11	1.89	0.53
1:B:78:LYS:HE3	1:B:78:LYS:N	2.06	0.53
1:D:164:LEU:CD1	1:D:177:LEU:HD11	2.38	0.53
1:C:150:ASN:HD22	1:C:152:PHE:H	1.57	0.53
1:H:263:TRP:CZ3	1:H:266:ASN:HB3	2.44	0.53
1:G:118:PRO:HD3	1:G:155:ASN:HD22	1.72	0.53
1:C:57:LEU:HB3	1:C:59:LEU:HD22	1.91	0.52
1:D:266:ASN:HD22	1:D:267:MET:H	1.57	0.52
1:F:238:LEU:O	1:F:238:LEU:HD13	2.09	0.52
1:C:295:HIS:CD2	1:D:260:ARG:HE	2.27	0.52
1:C:121:ASP:HB3	1:C:125:ARG:HH12	1.74	0.52
1:G:41:ASP:OD1	1:G:42:PRO:HD2	2.10	0.52
1:F:159:THR:HG22	1:F:161:ALA:N	2.21	0.52
1:C:263:TRP:CZ3	1:C:266:ASN:HB3	2.43	0.52
1:E:137:ALA:HB1	1:E:142:VAL:HG12	1.90	0.52
1:F:266:ASN:HD22	1:F:266:ASN:H	1.58	0.52
1:E:246:GLU:HG3	1:E:264:THR:HA	1.91	0.52
1:F:5:GLY:HA3	1:F:34:LEU:HD23	1.91	0.52
1:F:53:ARG:CG	1:F:53:ARG:NH1	2.60	0.52
1:F:104:ALA:HB1	1:F:178:HIS:CD2	2.45	0.51
1:F:266:ASN:H	1:F:266:ASN:ND2	2.07	0.51
1:E:123:TRP:NE1	1:G:296:LYS:HE3	2.26	0.51
1:F:238:LEU:HD12	1:F:238:LEU:N	2.14	0.51
1:G:147:GLU:HA	1:G:178:HIS:HB3	1.93	0.51
1:A:77:ASP:OD1	1:A:80:VAL:HG23	2.11	0.51
1:H:8:SER:O	1:H:11:TRP:N	2.42	0.51
1:C:182:PHE:CD1	1:C:212:ARG:HD2	2.45	0.51
1:F:114:GLN:NE2	1:F:114:GLN:HA	2.26	0.51
1:F:181:THR:HG22	1:F:208:GLY:O	2.10	0.51
1:H:102:LYS:HB3	1:H:143:THR:OG1	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:21:GLU:HA	1:F:24:LEU:HD22	1.93	0.51
1:H:9:PHE:CZ	1:H:38:SER:OG	2.64	0.51
1:E:83:ARG:HG2	1:E:83:ARG:HH11	1.75	0.51
1:F:52:LYS:HE2	1:F:56:ASP:OD2	2.11	0.50
1:G:72:ASP:OD1	1:G:74:SER:OG	2.29	0.50
1:A:74:SER:HB2	1:A:122:GLN:CG	2.40	0.50
1:C:67:LEU:HD21	1:C:88:LEU:HD13	1.94	0.50
1:B:266:ASN:ND2	1:B:266:ASN:N	2.59	0.50
1:H:209:GLU:CG	1:H:210:SER:N	2.75	0.50
1:B:70:ASP:OD1	1:B:70:ASP:O	2.30	0.50
1:E:3:ARG:HB3	1:E:33:ASP:CB	2.38	0.50
1:C:121:ASP:HB3	1:C:125:ARG:NH1	2.27	0.49
1:G:77:ASP:O	1:G:77:ASP:OD1	2.30	0.49
1:C:256:THR:OG1	1:C:258:ILE:CD1	2.61	0.49
1:B:287:LYS:O	1:B:291:VAL:HG23	2.13	0.49
1:E:245:SER:OG	1:E:261:ASN:HB3	2.12	0.49
1:G:244:SER:HB3	1:G:247:ILE:HB	1.93	0.49
1:B:21:GLU:OE2	1:B:53:ARG:NH1	2.46	0.49
1:A:21:GLU:HG2	1:A:53:ARG:HH12	1.78	0.49
1:G:159:THR:O	1:G:162:GLN:HB2	2.13	0.49
1:E:263:TRP:CZ3	1:E:266:ASN:HB3	2.48	0.48
1:H:94:LEU:O	1:H:98:LEU:HB2	2.13	0.48
1:E:43:ALA:O	1:E:44:ASP:HB2	2.12	0.48
1:A:64:SER:HA	1:A:104:ALA:O	2.14	0.48
1:C:296:LYS:HG2	1:C:297:PRO:HD2	1.95	0.48
1:A:260:ARG:HH11	1:B:295:HIS:CD2	2.30	0.48
1:G:3:ARG:NH2	1:G:60:GLY:HA3	2.09	0.48
1:A:38:SER:HA	1:A:64:SER:O	2.14	0.48
1:A:3:ARG:CD	1:A:33:ASP:OD1	2.59	0.48
1:E:83:ARG:CG	1:E:83:ARG:NH1	2.69	0.47
1:C:266:ASN:HD22	1:C:266:ASN:H	1.58	0.47
1:H:74:SER:HB3	1:H:122:GLN:CG	2.43	0.47
1:E:164:LEU:HD13	1:E:177:LEU:HD11	1.96	0.47
1:C:149:VAL:HG12	1:C:183:HIS:CD2	2.49	0.47
1:D:94:LEU:O	1:D:98:LEU:HB2	2.14	0.47
1:E:123:TRP:CE2	1:G:296:LYS:HE3	2.49	0.47
1:D:167:ILE:O	1:D:170:THR:OG1	2.30	0.47
1:E:103:VAL:HG12	1:E:107:LEU:HD21	1.97	0.47
1:B:9:PHE:HB3	1:B:248:VAL:HG12	1.96	0.47
1:C:149:VAL:O	1:C:158:ASN:HA	2.15	0.47
1:H:149:VAL:O	1:H:158:ASN:HA	2.13	0.47
1:C:147:GLU:HA	1:C:178:HIS:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:77:ASP:HB3	1:E:80:VAL:CG1	2.45	0.47
1:F:70:ASP:HB3	1:F:83:ARG:HE	1.80	0.47
1:G:73:ILE:HG22	1:G:84:GLY:HA3	1.97	0.47
1:D:70:ASP:HB2	1:D:83:ARG:HH21	1.80	0.47
1:H:167:ILE:HG21	1:H:201:LYS:HE2	1.96	0.47
1:E:167:ILE:O	1:E:170:THR:OG1	2.28	0.47
1:G:149:VAL:O	1:G:158:ASN:HA	2.14	0.47
1:C:212:ARG:HG2	1:C:243:PHE:HD2	1.79	0.47
1:A:72:ASP:C	1:A:72:ASP:OD1	2.52	0.47
1:E:249:ASP:O	1:E:253:SER:HB3	2.14	0.47
1:F:184:MET:HB3	1:F:191:VAL:HG12	1.95	0.47
1:H:240:PHE:CZ	1:H:242:SER:HB2	2.50	0.46
1:C:164:LEU:HD13	1:C:177:LEU:HD11	1.97	0.46
1:A:38:SER:OG	1:A:39:TYR:N	2.48	0.46
1:F:105:GLY:H	1:F:178:HIS:HD2	1.63	0.46
1:E:74:SER:HB2	1:E:122:GLN:HG2	1.97	0.46
1:F:178:HIS:HA	1:F:204:TYR:O	2.15	0.46
1:C:246:GLU:HG3	1:C:264:THR:HG22	1.98	0.46
1:H:104:ALA:O	1:H:107:LEU:HD11	2.16	0.46
1:G:245:SER:HB2	1:G:261:ASN:OD1	2.15	0.46
1:C:266:ASN:ND2	1:C:266:ASN:N	2.60	0.46
1:C:106:ILE:H	1:C:106:ILE:HD12	1.81	0.46
1:D:238:LEU:O	1:D:238:LEU:HD12	2.15	0.46
1:G:106:ILE:HD12	1:G:111:HIS:CG	2.51	0.46
1:F:254:LYS:HG2	1:F:254:LYS:H	1.50	0.46
1:G:77:ASP:OD1	1:G:79:ALA:HB3	2.16	0.45
1:F:164:LEU:HD13	1:F:177:LEU:HD11	1.97	0.45
1:D:28:ARG:NH1	1:D:29:ASP:OD1	2.48	0.45
1:A:21:GLU:CG	1:A:53:ARG:HH12	2.30	0.45
1:A:72:ASP:OD1	1:A:74:SER:OG	2.30	0.45
1:A:147:GLU:HA	1:A:178:HIS:HB3	1.98	0.45
1:D:40:LEU:HA	1:D:40:LEU:HD12	1.75	0.45
1:H:209:GLU:CG	1:H:210:SER:H	2.29	0.45
1:H:8:SER:O	1:H:11:TRP:HB2	2.17	0.45
1:A:3:ARG:HD2	1:A:3:ARG:HA	1.40	0.45
1:B:263:TRP:CE2	1:B:269:LEU:HD22	2.52	0.45
1:A:212:ARG:NH1	1:A:212:ARG:CG	2.53	0.45
1:G:111:HIS:O	1:G:255:LYS:CE	2.64	0.45
1:F:180:ASP:HB3	1:F:183:HIS:HD2	1.82	0.45
1:F:114:GLN:HG2	1:F:155:ASN:CG	2.37	0.44
1:H:30:ALA:HA	1:H:271:LYS:HG2	1.99	0.44
1:H:39:TYR:O	1:H:40:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:74:SER:HB2	1:B:122:GLN:HG2	1.99	0.44
1:G:46:ASP:OD2	1:G:49:ARG:HB2	2.17	0.44
1:C:243:PHE:HB3	1:C:258:ILE:HG12	1.99	0.44
1:D:215:LEU:O	1:D:272:HIS:HE1	2.01	0.44
1:A:254:LYS:HD3	1:D:115:VAL:O	2.17	0.44
1:F:65:ILE:HG13	1:F:66:GLY:N	2.32	0.44
1:H:178:HIS:HA	1:H:204:TYR:O	2.18	0.44
1:E:160:ALA:O	1:E:164:LEU:HB2	2.18	0.44
1:F:74:SER:HB3	1:F:126:SER:HB2	2.00	0.44
1:A:38:SER:O	1:A:39:TYR:HB2	2.18	0.43
1:H:199:ALA:HB1	1:H:232:ILE:HB	2.00	0.43
1:A:74:SER:HB2	1:A:122:GLN:HG3	1.99	0.43
1:C:251:ASN:O	1:C:255:LYS:HD2	2.19	0.43
1:F:121:ASP:O	1:F:125:ARG:HG3	2.18	0.43
1:G:106:ILE:CD1	1:G:111:HIS:CD2	3.00	0.43
1:D:50:LEU:HD13	1:D:98:LEU:HD11	2.01	0.43
1:H:274:ARG:HD2	1:H:274:ARG:HA	1.88	0.43
1:G:27:THR:HG23	1:G:32:PHE:HB2	2.01	0.43
1:A:74:SER:HB2	1:A:122:GLN:HG2	1.99	0.43
1:F:39:TYR:HA	1:F:65:ILE:HD12	1.99	0.43
1:C:147:GLU:HB2	1:C:178:HIS:ND1	2.33	0.43
1:B:64:SER:HA	1:B:104:ALA:O	2.19	0.43
1:B:94:LEU:O	1:B:98:LEU:HB2	2.18	0.43
1:C:67:LEU:HD21	1:C:88:LEU:CD1	2.48	0.43
1:H:149:VAL:HA	1:H:183:HIS:CG	2.53	0.43
1:F:210:SER:HB3	1:F:220:ILE:HG13	2.01	0.43
1:A:3:ARG:HB2	1:A:237:ASP:OD1	2.19	0.43
1:A:3:ARG:HB3	1:A:34:LEU:HB2	2.01	0.43
1:B:158:ASN:HD21	1:C:259:TRP:HD1	1.66	0.43
1:A:266:ASN:ND2	1:A:266:ASN:N	2.56	0.43
1:D:242:SER:HB3	1:D:269:LEU:HD21	2.01	0.43
1:E:250:GLU:HG2	1:E:254:LYS:HZ1	1.83	0.42
1:H:101:ARG:HG3	1:H:102:LYS:HG2	2.00	0.42
1:A:50:LEU:HD13	1:A:98:LEU:HD11	2.01	0.42
1:E:149:VAL:O	1:E:158:ASN:HA	2.19	0.42
1:B:250:GLU:O	1:B:254:LYS:HE3	2.19	0.42
1:E:42:PRO:HG3	1:E:94:LEU:HD22	2.01	0.42
1:H:252:LEU:O	1:H:256:THR:OG1	2.36	0.42
1:D:103:VAL:HG23	1:D:142:VAL:CG1	2.49	0.42
1:D:244:SER:O	1:D:248:VAL:HG22	2.20	0.42
1:D:276:PHE:CE1	3:D:1002:MPD:H12	2.53	0.42
1:A:67:LEU:HD21	1:A:88:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:167:ILE:HG12	1:G:175:ILE:HG22	2.02	0.42
1:C:211:HIS:O	1:C:212:ARG:HB2	2.20	0.42
1:B:104:ALA:HB1	1:B:178:HIS:CD2	2.55	0.42
1:G:3:ARG:CB	1:G:237:ASP:OD1	2.66	0.42
1:A:193:LEU:HD12	1:A:193:LEU:HA	1.85	0.42
1:G:290:LEU:HD11	1:H:262:LEU:HG	2.01	0.42
1:E:159:THR:O	1:E:162:GLN:HB2	2.20	0.41
1:B:9:PHE:HB2	1:B:243:PHE:CE1	2.56	0.41
1:F:118:PRO:CD	1:G:259:TRP:HB3	2.50	0.41
1:E:67:LEU:HB2	1:E:109:ALA:O	2.20	0.41
1:E:83:ARG:HG2	1:E:83:ARG:NH1	2.33	0.41
1:E:215:LEU:HD13	1:E:240:PHE:HE1	1.85	0.41
1:G:115:VAL:HG13	1:G:116:GLU:HG2	2.03	0.41
1:A:21:GLU:HG2	1:A:53:ARG:NH1	2.35	0.41
1:H:199:ALA:CB	1:H:232:ILE:HB	2.50	0.41
1:H:83:ARG:O	1:H:87:ILE:HG22	2.20	0.41
1:G:113:LEU:HD13	1:G:152:PHE:HA	2.01	0.41
1:G:215:LEU:HD13	1:G:240:PHE:CE1	2.55	0.41
1:C:159:THR:CG2	1:C:161:ALA:HB3	2.50	0.41
1:A:245:SER:CB	1:A:261:ASN:HD21	2.30	0.41
1:C:249:ASP:HB3	1:C:251:ASN:H	1.85	0.41
1:F:296:LYS:HA	1:F:297:PRO:HD3	1.94	0.41
1:A:214:PHE:CE2	1:A:269:LEU:HA	2.55	0.41
1:E:106:ILE:HD13	1:E:111:HIS:CG	2.56	0.41
1:G:42:PRO:C	1:G:44:ASP:N	2.73	0.40
1:B:198:ALA:O	1:B:199:ALA:C	2.59	0.40
1:H:67:LEU:HA	1:H:68:PRO:HD3	1.97	0.40
1:F:191:VAL:HG23	1:F:192:GLY:N	2.37	0.40
1:G:96:ARG:HG2	1:G:97:ASP:N	2.36	0.40
1:C:65:ILE:HD13	1:C:91:THR:HG21	2.03	0.40
1:E:123:TRP:CE3	1:G:297:PRO:HD2	2.56	0.40
1:D:147:GLU:HA	1:D:178:HIS:HB3	2.02	0.40
1:G:209:GLU:HG3	1:G:210:SER:N	2.35	0.40
1:A:274:ARG:HA	1:A:274:ARG:HD2	1.87	0.40
1:F:1:MET:HB3	1:F:1:MET:HE3	1.69	0.40
1:B:214:PHE:CE1	1:B:269:LEU:HA	2.57	0.40
1:G:75:SER:OG	1:G:80:VAL:HG21	2.22	0.40
1:H:46:ASP:HB2	1:H:49:ARG:HB3	2.03	0.40
1:E:149:VAL:HA	1:E:183:HIS:CG	2.56	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	295/297 (99%)	292 (99%)	3 (1%)	0	100	100
1	B	295/297 (99%)	285 (97%)	10 (3%)	0	100	100
1	C	295/297 (99%)	289 (98%)	6 (2%)	0	100	100
1	D	295/297 (99%)	293 (99%)	2 (1%)	0	100	100
1	E	295/297 (99%)	291 (99%)	4 (1%)	0	100	100
1	F	295/297 (99%)	290 (98%)	5 (2%)	0	100	100
1	G	295/297 (99%)	291 (99%)	4 (1%)	0	100	100
1	H	295/297 (99%)	287 (97%)	8 (3%)	0	100	100
All	All	2360/2376 (99%)	2318 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	225/225 (100%)	198 (88%)	27 (12%)	7	17
1	B	225/225 (100%)	200 (89%)	25 (11%)	9	20
1	C	225/225 (100%)	202 (90%)	23 (10%)	11	24
1	D	225/225 (100%)	199 (88%)	26 (12%)	8	18
1	E	225/225 (100%)	208 (92%)	17 (8%)	19	41
1	F	225/225 (100%)	205 (91%)	20 (9%)	14	31
1	G	225/225 (100%)	197 (88%)	28 (12%)	7	16
1	H	225/225 (100%)	197 (88%)	28 (12%)	7	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1800/1800 (100%)	1606 (89%)	194 (11%)	9 21

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	18	SER
1	A	21	GLU
1	A	22	ARG
1	A	24	LEU
1	A	38	SER
1	A	50	LEU
1	A	52	LYS
1	A	53	ARG
1	A	56	ASP
1	A	57	LEU
1	A	59	LEU
1	A	77	ASP
1	A	88	LEU
1	A	101	ARG
1	A	115	VAL
1	A	159	THR
1	A	164	LEU
1	A	193	LEU
1	A	212	ARG
1	A	215	LEU
1	A	217	THR
1	A	249	ASP
1	A	253	SER
1	A	266	ASN
1	A	286	ARG
1	A	287	LYS
1	B	1	MET
1	B	8	SER
1	B	20	LEU
1	B	22	ARG
1	B	28	ARG
1	B	38	SER
1	B	53	ARG
1	B	59	LEU
1	B	70	ASP
1	B	78	LYS

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Mol	Chain	Res	Type
1	B	102	LYS
1	B	114	GLN
1	B	142	VAL
1	B	146	LEU
1	B	159	THR
1	B	164	LEU
1	B	178	HIS
1	B	193	LEU
1	B	201	LYS
1	B	211	HIS
1	B	212	ARG
1	B	215	LEU
1	B	255	LYS
1	B	266	ASN
1	B	267	MET
1	C	20	LEU
1	C	22	ARG
1	C	24	LEU
1	C	57	LEU
1	C	59	LEU
1	C	77	ASP
1	C	78	LYS
1	C	88	LEU
1	C	90	GLN
1	C	91	THR
1	C	98	LEU
1	C	146	LEU
1	C	159	THR
1	C	193	LEU
1	C	211	HIS
1	C	212	ARG
1	C	215	LEU
1	C	246	GLU
1	C	262	LEU
1	C	266	ASN
1	C	274	ARG
1	C	281	LEU
1	C	289	GLU
1	D	20	LEU
1	D	34	LEU
1	D	38	SER
1	D	40	LEU

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Mol	Chain	Res	Type
1	D	50	LEU
1	D	53	ARG
1	D	65	ILE
1	D	83	ARG
1	D	88	LEU
1	D	107	LEU
1	D	120	ARG
1	D	146	LEU
1	D	159	THR
1	D	164	LEU
1	D	193	LEU
1	D	211	HIS
1	D	212	ARG
1	D	215	LEU
1	D	249	ASP
1	D	260	ARG
1	D	264	THR
1	D	266	ASN
1	D	271	LYS
1	D	274	ARG
1	D	281	LEU
1	D	296	LYS
1	E	1	MET
1	E	3	ARG
1	E	50	LEU
1	E	57	LEU
1	E	59	LEU
1	E	80	VAL
1	E	83	ARG
1	E	88	LEU
1	E	116	GLU
1	E	159	THR
1	E	193	LEU
1	E	215	LEU
1	E	254	LYS
1	E	255	LYS
1	E	264	THR
1	E	266	ASN
1	E	285	ARG
1	F	1	MET
1	F	24	LEU
1	F	28	ARG

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Mol	Chain	Res	Type
1	F	52	LYS
1	F	53	ARG
1	F	59	LEU
1	F	65	ILE
1	F	98	LEU
1	F	102	LYS
1	F	107	LEU
1	F	108	SER
1	F	114	GLN
1	F	146	LEU
1	F	178	HIS
1	F	193	LEU
1	F	212	ARG
1	F	215	LEU
1	F	238	LEU
1	F	253	SER
1	F	262	LEU
1	G	1	MET
1	G	3	ARG
1	G	21	GLU
1	G	28	ARG
1	G	33	ASP
1	G	46	ASP
1	G	49	ARG
1	G	50	LEU
1	G	77	ASP
1	G	80	VAL
1	G	96	ARG
1	G	107	LEU
1	G	114	GLN
1	G	149	VAL
1	G	159	THR
1	G	164	LEU
1	G	193	LEU
1	G	211	HIS
1	G	212	ARG
1	G	245	SER
1	G	246	GLU
1	G	258	ILE
1	G	265	ASP
1	G	266	ASN
1	G	267	MET

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Mol	Chain	Res	Type
1	G	274	ARG
1	G	292	SER
1	G	294	ARG
1	H	1	MET
1	H	3	ARG
1	H	22	ARG
1	H	28	ARG
1	H	29	ASP
1	H	34	LEU
1	H	45	VAL
1	H	46	ASP
1	H	47	ILE
1	H	56	ASP
1	H	87	ILE
1	H	102	LYS
1	H	107	LEU
1	H	113	LEU
1	H	115	VAL
1	H	146	LEU
1	H	159	THR
1	H	164	LEU
1	H	191	VAL
1	H	201	LYS
1	H	211	HIS
1	H	215	LEU
1	H	245	SER
1	H	254	LYS
1	H	255	LYS
1	H	260	ARG
1	H	266	ASN
1	H	274	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	17	GLN
1	A	145	ASN
1	A	158	ASN
1	A	266	ASN
1	B	7	HIS
1	B	158	ASN

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Mol	Chain	Res	Type
1	B	178	HIS
1	B	266	ASN
1	B	272	HIS
1	B	295	HIS
1	C	150	ASN
1	C	158	ASN
1	C	266	ASN
1	C	295	HIS
1	D	7	HIS
1	D	158	ASN
1	D	266	ASN
1	D	295	HIS
1	E	266	ASN
1	F	7	HIS
1	F	114	GLN
1	F	178	HIS
1	F	266	ASN
1	G	183	HIS
1	G	197	HIS
1	G	251	ASN
1	G	266	ASN
1	G	272	HIS
1	H	7	HIS
1	H	17	GLN
1	H	158	ASN
1	H	211	HIS
1	H	266	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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	MPD	A	1002	-	7,7,7	0.20	0	10,10,10	0.39	0
3	MPD	B	1002	-	7,7,7	0.32	0	10,10,10	0.52	0
3	MPD	D	1002	-	7,7,7	0.26	0	10,10,10	0.54	0
3	MPD	E	1002	-	7,7,7	0.25	0	10,10,10	0.34	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	MPD	A	1002	-	-	0/5/5/5	0/0/0/0
3	MPD	B	1002	-	-	0/5/5/5	0/0/0/0
3	MPD	D	1002	-	-	0/5/5/5	0/0/0/0
3	MPD	E	1002	-	-	0/5/5/5	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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, 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	297/297 (100%)	-0.34	0 100 100	19, 36, 60, 79	0
1	B	297/297 (100%)	-0.31	0 100 100	18, 36, 60, 87	0
1	C	297/297 (100%)	-0.42	1 (0%) 91 95	20, 33, 52, 65	0
1	D	297/297 (100%)	-0.51	0 100 100	18, 31, 58, 78	0
1	E	297/297 (100%)	-0.25	1 (0%) 91 95	26, 44, 72, 92	0
1	F	297/297 (100%)	-0.05	5 (1%) 67 73	26, 49, 72, 96	0
1	G	297/297 (100%)	0.48	23 (7%) 13 14	38, 67, 100, 130	0
1	H	297/297 (100%)	0.28	17 (5%) 23 25	36, 59, 99, 123	0
All	All	2376/2376 (100%)	-0.14	47 (1%) 62 68	18, 43, 84, 130	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	40	LEU	5.9
1	G	1	MET	5.2
1	G	39	TYR	5.2
1	H	39	TYR	4.8
1	H	42	PRO	4.7
1	H	43	ALA	4.4
1	G	246	GLU	3.6
1	G	43	ALA	3.2
1	G	44	ASP	3.2
1	H	82	ALA	3.1
1	H	14	SER	3.1
1	G	54	ILE	3.0
1	G	101	ARG	2.9
1	H	139	ALA	2.9
1	G	18	SER	2.9
1	G	41	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	58	GLY	2.8
1	F	76	ALA	2.7
1	H	70	ASP	2.7
1	G	30	ALA	2.6
1	G	52	LYS	2.6
1	F	79	ALA	2.6
1	G	2	ALA	2.6
1	F	1	MET	2.5
1	F	69	ALA	2.5
1	E	44	ASP	2.4
1	H	38	SER	2.4
1	H	40	LEU	2.4
1	H	47	ILE	2.4
1	H	49	ARG	2.4
1	H	1	MET	2.4
1	G	250	GLU	2.4
1	G	99	GLY	2.3
1	F	78	LYS	2.3
1	G	123	TRP	2.3
1	H	115	VAL	2.3
1	G	42	PRO	2.3
1	H	52	LYS	2.2
1	G	247	ILE	2.2
1	G	115	VAL	2.2
1	H	289	GLU	2.2
1	H	297	PRO	2.2
1	H	246	GLU	2.2
1	G	141	GLY	2.1
1	C	200	GLY	2.0
1	G	95	THR	2.0
1	G	29	ASP	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MPD	D	1002	8/8	0.26	8.63	62,66,76,80	0
3	MPD	A	1002	8/8	0.24	6.91	59,61,67,70	0
3	MPD	B	1002	8/8	0.25	4.53	46,50,53,56	0
3	MPD	E	1002	8/8	0.24	2.42	57,60,64,68	0
2	MN	E	1001	1/1	0.17	-0.33	33,33,33,33	0
2	MN	F	1001	1/1	0.19	-0.90	41,41,41,41	0
2	MN	A	1001	1/1	0.15	-1.74	21,21,21,21	0
2	MN	D	1001	1/1	0.16	-2.35	22,22,22,22	0
2	MN	H	1001	1/1	0.11	-2.63	43,43,43,43	0
2	MN	B	1001	1/1	0.13	-3.69	26,26,26,26	0
2	MN	C	1001	1/1	0.16	-4.05	26,26,26,26	0
2	MN	G	1001	1/1	0.14	-4.11	50,50,50,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.