



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:37 AM UTC

PDB ID : 3OWQ / pdb_00003owq
Title : X-Ray Structure of Lin1025 protein from *Listeria innocua*, Northeast Structural Genomics Consortium Target LkR164
Authors : Kuzin, A.; Su, M.; Lew, S.; Seetharaman, J.; Patel, P.; Xiao, R.; Ciccocanti, C.; Lee, D.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2010-09-20
Resolution : 2.61 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

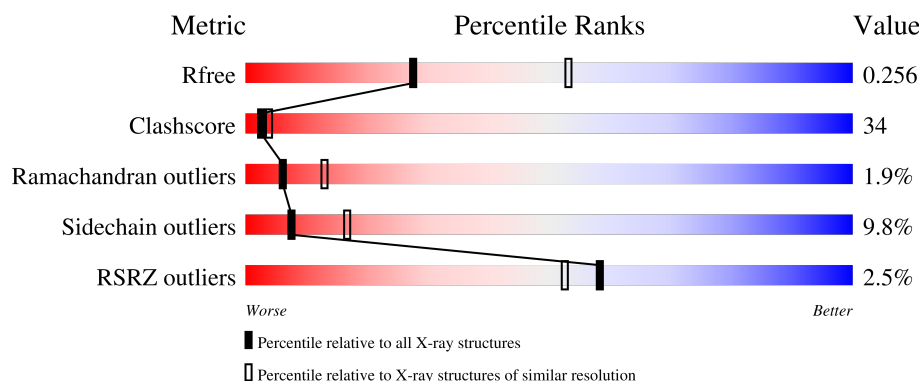
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	321	2% 39% 29% 5% 26%
1	B	321	2% 33% 34% 6% 27%
1	C	321	% 31% 36% 7% 26%
1	D	321	2% 34% 34% 6% 26%

2 Entry composition [i](#)

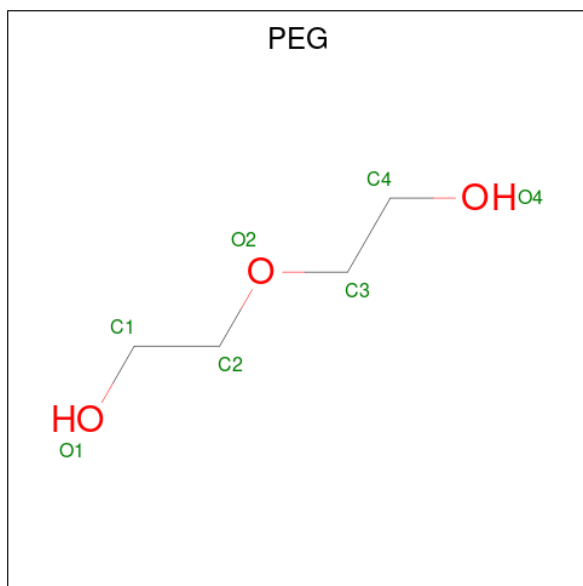
There are 3 unique types of molecules in this entry. The entry contains 7361 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lin1025 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	Se	0	0	0
			1832	1146	305	372	9			
1	B	233	Total	C	N	O	Se	0	0	0
			1790	1117	301	363	9			
1	C	237	Total	C	N	O	Se	0	0	0
			1830	1148	305	368	9			
1	D	237	Total	C	N	O	Se	0	0	0
			1840	1155	305	371	9			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			7	4	3		

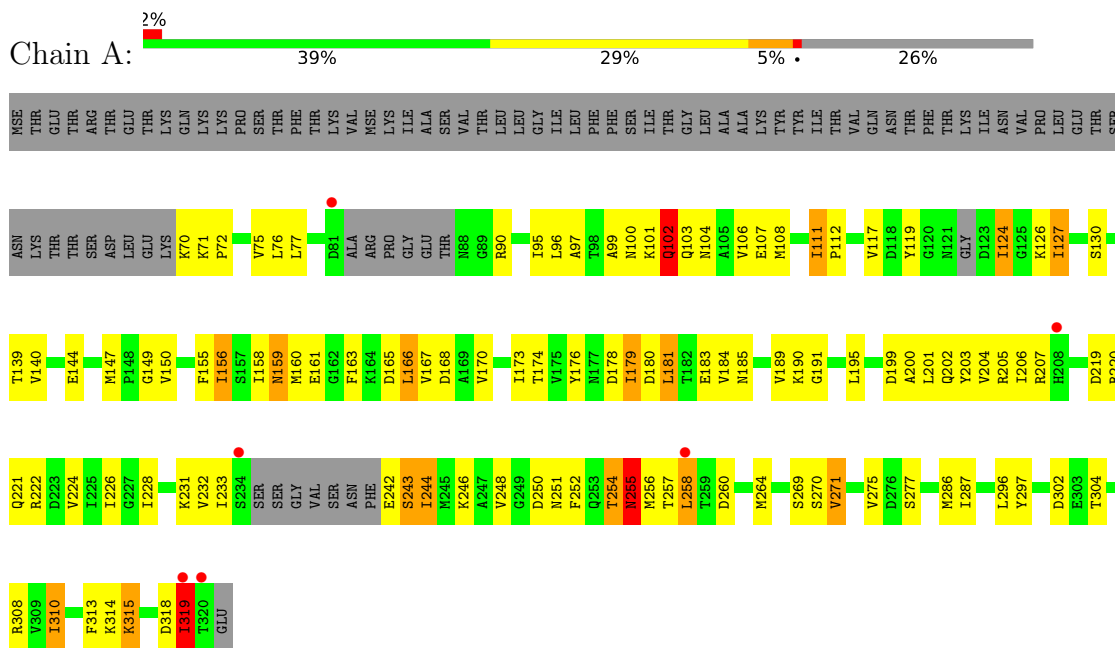
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	12	Total	O	0	0
			12	12		
3	C	11	Total	O	0	0
			11	11		
3	D	17	Total	O	0	0
			17	17		

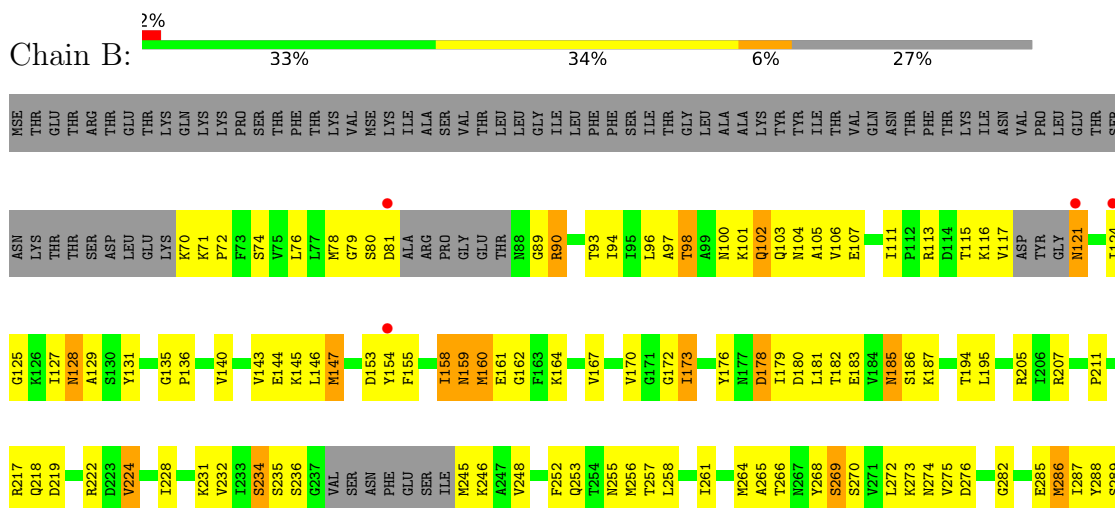
3 Residue-property plots

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

• Molecule 1: Lin1025 protein

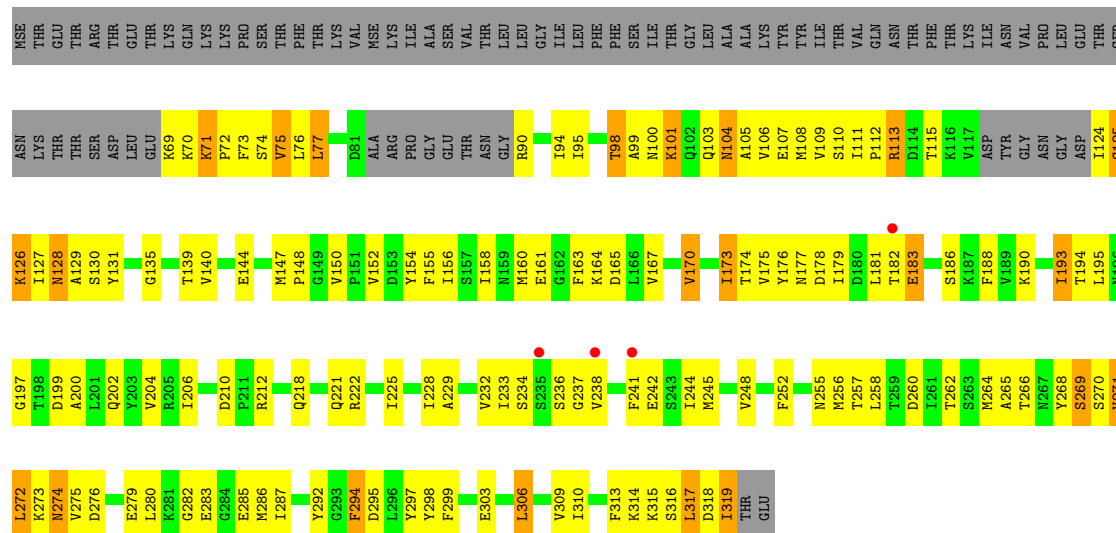


• Molecule 1: Lin1025 protein

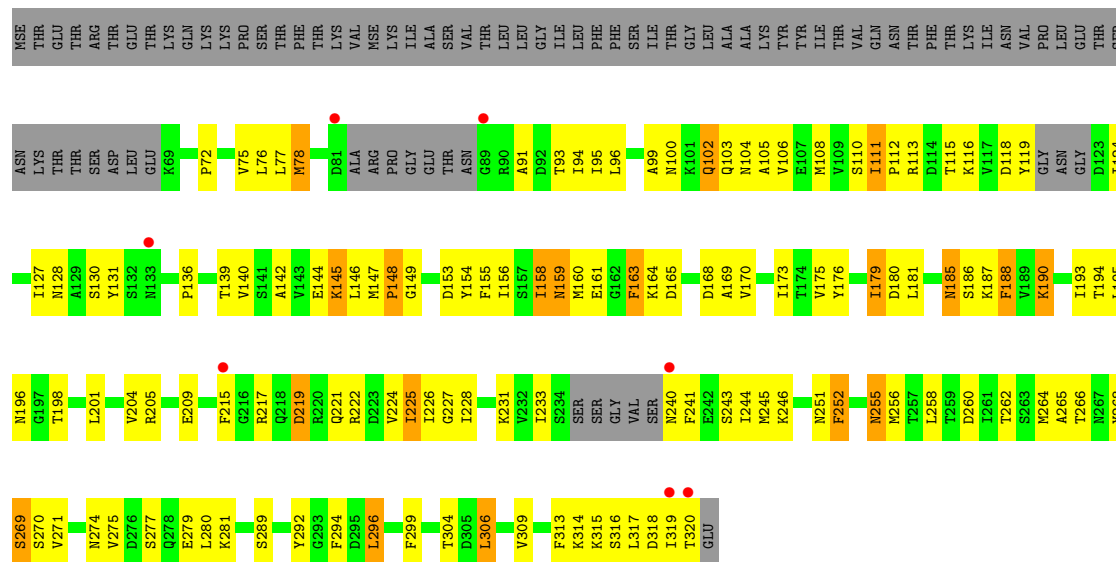




• Molecule 1: Lin1025 protein



• Molecule 1: Lin1025 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.51Å 157.04Å 57.28Å 90.00° 98.38° 90.00°	Depositor
Resolution (Å)	28.33 – 2.61 28.33 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.3 (28.33-2.61) 99.3 (28.33-2.61)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.225 , 0.260 0.222 , 0.256	Depositor DCC
R_{free} test set	1515 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.106 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7361	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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

5.1 Standard geometry

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

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	0/1846	1.01	7/2474 (0.3%)
1	B	0.48	0/1804	1.03	10/2417 (0.4%)
1	C	0.49	0/1845	0.99	10/2472 (0.4%)
1	D	0.49	0/1855	1.02	15/2485 (0.6%)
All	All	0.49	0/7350	1.01	42/9848 (0.4%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	VAL	N-CA-C	11.78	120.49	108.95
1	C	150	VAL	N-CA-C	9.18	118.97	108.96
1	D	110	SER	CA-C-N	-7.64	117.09	122.59
1	D	110	SER	C-N-CA	-7.64	117.09	122.59
1	A	119	TYR	N-CA-C	-7.33	104.59	113.97
1	A	179	ILE	N-CA-C	7.00	118.56	108.48
1	D	316	SER	N-CA-C	-6.94	103.77	111.82
1	C	126	LYS	N-CA-C	6.68	120.17	110.28
1	D	147	MSE	CA-C-N	6.51	127.97	119.84
1	D	147	MSE	C-N-CA	6.51	127.97	119.84
1	A	246	LYS	N-CA-C	-6.44	105.43	113.55
1	D	225	ILE	N-CA-C	-6.09	104.81	110.53
1	C	303	GLU	N-CA-C	6.07	118.69	111.71
1	D	317	LEU	N-CA-C	-5.96	98.10	110.80
1	B	147	MSE	CA-C-N	5.95	127.28	119.84
1	B	147	MSE	C-N-CA	5.95	127.28	119.84
1	B	224	VAL	N-CA-C	5.92	116.66	110.62
1	C	71	LYS	CA-C-N	5.92	126.27	119.93
1	C	71	LYS	C-N-CA	5.92	126.27	119.93
1	A	255	ASN	N-CA-C	-5.86	106.09	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	161	GLU	N-CA-C	-5.83	104.56	111.03
1	D	306	LEU	N-CA-C	-5.79	104.87	111.07
1	B	286	MSE	N-CA-C	-5.78	100.28	109.76
1	C	125	GLY	N-CA-C	5.76	126.84	113.18
1	C	160	MSE	N-CA-C	5.62	118.13	111.33
1	D	163	PHE	N-CA-C	-5.42	105.01	111.03
1	D	179	ILE	N-CA-C	5.42	115.69	108.27
1	A	250	ASP	N-CA-C	5.39	118.66	111.75
1	C	163	PHE	N-CA-C	-5.22	105.23	111.03
1	D	153	ASP	N-CA-C	5.17	116.60	111.07
1	D	215	PHE	N-CA-C	-5.12	105.82	111.71
1	B	234	SER	CB-CA-C	-5.12	108.00	114.40
1	B	160	MSE	N-CA-C	5.12	116.86	111.28
1	D	209	GLU	N-CA-C	5.11	119.00	112.87
1	A	159	ASN	N-CA-C	-5.10	102.45	110.36
1	B	293	GLY	N-CA-C	-5.10	105.22	114.46
1	C	135	GLY	CA-C-N	5.10	126.21	119.84
1	C	135	GLY	C-N-CA	5.10	126.21	119.84
1	B	144	GLU	N-CA-C	-5.06	106.96	113.23
1	D	159	ASN	N-CA-C	-5.05	102.52	110.36
1	B	135	GLY	CA-C-N	5.04	125.31	119.47
1	B	135	GLY	C-N-CA	5.04	125.31	119.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1832	0	1803	120	0
1	B	1790	0	1763	132	0
1	C	1830	0	1817	132	0
1	D	1840	0	1816	127	0
2	B	7	0	10	0	0
2	C	7	0	10	1	0
2	D	7	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	0	0	0
3	B	12	0	0	1	0
3	C	11	0	0	0	0
3	D	17	0	0	0	0
All	All	7361	0	7229	500	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 34.

All (500) 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:111:ILE:HD11	1:A:127:ILE:HG21	1.31	1.11
1:D:106:VAL:HG22	1:D:271:VAL:HG12	1.34	1.05
1:D:190:LYS:H	1:D:190:LYS:HD3	1.20	1.03
1:B:116:LYS:HG3	1:B:124:ILE:HD11	1.41	0.99
1:C:241:PHE:HE1	1:C:258:LEU:HG	1.22	0.99
1:A:124:ILE:HD13	1:A:124:ILE:H	1.26	0.98
1:B:159:ASN:HD21	1:B:162:GLY:H	1.14	0.96
1:C:113:ARG:H	1:C:113:ARG:HE	1.02	0.95
1:B:72:PRO:HG3	1:B:100:ASN:CG	1.92	0.95
1:C:167:VAL:HG21	1:C:197:GLY:HA2	1.52	0.92
1:D:185:ASN:HD22	1:D:186:SER:N	1.69	0.89
1:D:160:MSE:HG3	1:D:205:ARG:HH21	1.39	0.88
1:A:108:MSE:HE1	1:A:222:ARG:HG3	1.54	0.88
1:D:281:LYS:HE2	1:D:281:LYS:HA	1.55	0.87
1:D:111:ILE:HD11	1:D:127:ILE:HG12	1.53	0.87
1:B:159:ASN:ND2	1:B:162:GLY:H	1.73	0.86
1:B:306:LEU:O	1:B:310:ILE:HD13	1.75	0.86
1:B:72:PRO:HB3	1:B:100:ASN:HB2	1.56	0.86
1:C:241:PHE:CE1	1:C:258:LEU:HG	2.10	0.85
1:A:242:GLU:HG2	1:A:244:ILE:HG22	1.57	0.85
1:C:173:ILE:HD11	1:C:228:ILE:HA	1.60	0.84
1:C:113:ARG:H	1:C:113:ARG:NE	1.75	0.83
1:D:221:GLN:O	1:D:225:ILE:HG12	1.78	0.83
1:A:242:GLU:HG3	1:A:243:SER:H	1.44	0.82
1:D:222:ARG:HH22	1:D:275:VAL:HG13	1.43	0.82
1:B:147:MSE:HG2	1:B:310:ILE:HD11	1.60	0.82
1:A:108:MSE:HE3	1:A:277:SER:HB3	1.59	0.82
1:A:184:VAL:HG21	1:A:206:ILE:HD12	1.60	0.81
1:B:159:ASN:C	1:B:159:ASN:HD22	1.87	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASP:HB2	1:A:190:LYS:HE3	1.62	0.81
1:B:145:LYS:NZ	1:B:145:LYS:HB3	1.94	0.81
1:A:126:LYS:HE3	1:A:297:TYR:O	1.81	0.81
1:C:286:MSE:HB3	1:C:295:ASP:HB3	1.63	0.81
1:D:140:VAL:O	1:D:144:GLU:HG3	1.79	0.81
1:D:240:ASN:O	1:D:244:ILE:HD12	1.81	0.80
1:A:184:VAL:HG11	1:A:206:ILE:HD11	1.64	0.80
1:A:102:GLN:H	1:A:102:GLN:NE2	1.81	0.78
1:D:314:LYS:HD3	1:D:319:ILE:HD12	1.66	0.77
1:C:112:PRO:HA	1:C:113:ARG:HH21	1.50	0.77
1:D:106:VAL:HB	1:D:275:VAL:HG23	1.64	0.77
1:A:242:GLU:HG3	1:A:243:SER:N	1.99	0.77
1:A:170:VAL:CG1	1:A:231:LYS:HB3	2.14	0.77
1:C:176:TYR:HE2	1:C:178:ASP:HB3	1.50	0.77
1:D:222:ARG:NH2	1:D:275:VAL:HG13	2.00	0.77
1:D:106:VAL:CG2	1:D:271:VAL:HG12	2.14	0.76
1:B:147:MSE:HB3	1:B:310:ILE:HG13	1.65	0.76
1:D:185:ASN:ND2	1:D:187:LYS:H	1.84	0.76
1:B:140:VAL:O	1:B:143:VAL:HG12	1.85	0.76
1:C:101:LYS:HE2	1:C:270:SER:OG	1.84	0.76
1:A:255:ASN:HD22	1:A:256:MSE:N	1.85	0.75
1:D:173:ILE:HD11	1:D:228:ILE:HA	1.69	0.75
1:B:100:ASN:ND2	1:B:102:GLN:HB2	2.01	0.75
1:C:285:GLU:HG3	1:C:287:ILE:HD11	1.68	0.74
1:C:115:THR:HA	1:C:299:PHE:HB3	1.70	0.74
1:C:233:ILE:HG22	1:C:265:ALA:HB1	1.69	0.74
1:B:116:LYS:HG3	1:B:124:ILE:CD1	2.17	0.74
1:D:268:TYR:O	1:D:271:VAL:HG23	1.87	0.74
1:C:286:MSE:O	1:C:287:ILE:HD13	1.87	0.74
1:D:185:ASN:HD22	1:D:185:ASN:C	1.95	0.74
1:A:160:MSE:HG3	1:A:205:ARG:HH21	1.54	0.73
1:A:258:LEU:HD12	1:A:258:LEU:H	1.54	0.73
1:C:113:ARG:HE	1:C:113:ARG:N	1.84	0.72
1:B:185:ASN:C	1:B:185:ASN:HD22	1.97	0.72
1:D:160:MSE:HG3	1:D:205:ARG:NH2	2.04	0.72
1:B:167:VAL:HG22	1:B:228:ILE:HD11	1.70	0.72
1:A:242:GLU:CG	1:A:243:SER:N	2.53	0.71
1:B:270:SER:O	1:B:273:LYS:HG2	1.91	0.71
1:D:190:LYS:HD3	1:D:190:LYS:N	2.03	0.71
1:A:106:VAL:HG23	1:A:271:VAL:O	1.91	0.71
1:D:113:ARG:HG3	1:D:128:ASN:HB3	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:VAL:HG13	1:C:262:THR:HG23	1.73	0.71
1:C:106:VAL:CG2	1:C:271:VAL:HG13	2.21	0.70
1:A:108:MSE:HE2	1:A:275:VAL:CG1	2.21	0.70
1:A:106:VAL:HB	1:A:275:VAL:HG22	1.73	0.70
1:D:94:ILE:C	1:D:95:ILE:HD12	2.16	0.70
1:C:90:ARG:HB2	1:C:131:TYR:HB3	1.73	0.69
1:D:190:LYS:H	1:D:190:LYS:CD	2.00	0.69
1:A:206:ILE:HB	1:A:220:ARG:NH1	2.07	0.69
1:B:98:THR:OG1	1:B:317:LEU:HD11	1.93	0.69
1:C:111:ILE:HA	1:C:280:LEU:HD21	1.73	0.69
1:C:167:VAL:CG2	1:C:197:GLY:HA2	2.22	0.69
1:A:104:ASN:HD21	1:A:270:SER:HB3	1.58	0.69
1:A:195:LEU:HD22	1:A:199:ASP:HB3	1.74	0.68
1:C:72:PRO:HG3	1:C:100:ASN:OD1	1.92	0.68
1:D:163:PHE:HZ	1:D:224:VAL:HG11	1.59	0.68
1:D:76:LEU:HD23	1:D:78:MSE:HE2	1.74	0.68
1:B:117:VAL:HG12	1:B:125:GLY:O	1.93	0.67
1:C:176:TYR:HE1	1:D:269:SER:HG	1.42	0.67
1:A:314:LYS:HB3	1:A:319:ILE:CG2	2.25	0.67
1:B:136:PRO:O	1:B:140:VAL:HG23	1.96	0.66
1:C:126:LYS:HE2	1:C:297:TYR:O	1.95	0.66
1:B:117:VAL:HG12	1:B:125:GLY:C	2.20	0.66
1:C:176:TYR:CE2	1:C:178:ASP:HB3	2.30	0.65
1:B:313:PHE:O	1:B:317:LEU:HD13	1.96	0.65
1:D:131:TYR:HE1	1:D:136:PRO:HG3	1.61	0.65
1:A:124:ILE:HD13	1:A:124:ILE:N	2.06	0.65
1:A:170:VAL:HG12	1:A:231:LYS:HB3	1.78	0.65
1:A:124:ILE:H	1:A:124:ILE:CD1	2.06	0.65
1:C:74:SER:OG	1:C:152:VAL:HA	1.97	0.65
1:D:260:ASP:O	1:D:264:MSE:HB2	1.96	0.65
1:C:106:VAL:HG23	1:C:271:VAL:HG13	1.79	0.64
1:D:170:VAL:HG12	1:D:170:VAL:O	1.96	0.64
1:B:173:ILE:HD11	1:B:228:ILE:HA	1.78	0.64
1:C:292:TYR:HB3	1:C:294:PHE:CE1	2.32	0.64
1:A:159:ASN:ND2	1:A:161:GLU:HB2	2.12	0.64
1:A:319:ILE:HD13	1:A:319:ILE:H	1.61	0.64
1:C:306:LEU:O	1:C:310:ILE:HG13	1.98	0.64
1:A:286:MSE:C	1:A:287:ILE:HD12	2.22	0.64
1:A:95:ILE:HD11	1:A:221:GLN:OE1	1.98	0.64
1:A:258:LEU:HD12	1:A:258:LEU:N	2.13	0.64
1:C:125:GLY:CA	1:C:298:TYR:HE1	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:VAL:HG22	1:D:271:VAL:CG1	2.20	0.63
1:B:145:LYS:HB3	1:B:145:LYS:HZ2	1.62	0.63
1:B:248:VAL:CG1	1:B:252:PHE:HB2	2.28	0.63
1:A:70:LYS:HD2	1:A:101:LYS:HG2	1.80	0.63
1:A:206:ILE:HB	1:A:220:ARG:CZ	2.29	0.63
1:D:72:PRO:HG2	1:D:100:ASN:ND2	2.12	0.63
1:A:179:ILE:HG23	1:A:181:LEU:HD13	1.79	0.63
1:B:185:ASN:HD22	1:B:186:SER:N	1.97	0.62
1:A:184:VAL:HG21	1:A:206:ILE:CD1	2.30	0.62
1:C:260:ASP:O	1:C:264:MSE:HB2	1.99	0.62
1:B:248:VAL:HG11	1:B:252:PHE:HB2	1.81	0.62
1:C:179:ILE:O	1:C:181:LEU:HG	1.99	0.62
1:C:200:ALA:O	1:C:204:VAL:HG23	1.99	0.62
1:B:72:PRO:HG3	1:B:100:ASN:ND2	2.14	0.62
1:C:269:SER:HG	1:D:176:TYR:HE1	1.45	0.62
1:B:160:MSE:HG3	1:B:205:ARG:NH2	2.14	0.62
1:A:226:ILE:HD11	1:A:275:VAL:HG11	1.82	0.62
1:B:308:ARG:HH11	1:B:308:ARG:HG2	1.65	0.61
1:D:115:THR:HA	1:D:299:PHE:HB3	1.82	0.61
1:A:158:ILE:O	1:A:158:ILE:HD12	2.00	0.61
1:D:204:VAL:CG1	1:D:224:VAL:HG21	2.31	0.61
1:C:158:ILE:O	1:C:158:ILE:HD12	2.01	0.61
1:C:113:ARG:HB2	1:C:128:ASN:HB3	1.83	0.61
1:B:185:ASN:ND2	1:B:187:LYS:H	1.99	0.61
1:C:286:MSE:HB3	1:C:295:ASP:CB	2.32	0.60
1:C:105:ALA:O	1:C:271:VAL:HG22	2.02	0.60
1:B:207:ARG:HH12	1:B:217:ARG:NH1	2.00	0.60
1:C:319:ILE:C	1:C:319:ILE:HD13	2.26	0.60
1:B:246:LYS:NZ	1:C:202:GLN:HE21	2.00	0.60
1:D:185:ASN:HD21	1:D:187:LYS:HG3	1.66	0.59
1:B:124:ILE:HD12	1:B:125:GLY:H	1.67	0.59
1:A:170:VAL:HG12	1:A:170:VAL:O	2.03	0.59
1:A:96:LEU:HD12	1:A:313:PHE:CZ	2.38	0.59
1:D:76:LEU:HD12	1:D:95:ILE:O	2.02	0.58
1:B:179:ILE:O	1:B:181:LEU:HG	2.03	0.58
1:C:125:GLY:HA3	1:C:298:TYR:HE1	1.68	0.58
1:C:238:VAL:HG12	1:C:238:VAL:O	2.02	0.58
1:A:163:PHE:HZ	1:A:224:VAL:HG11	1.68	0.58
1:B:76:LEU:HD22	1:B:143:VAL:HG11	1.85	0.58
1:B:105:ALA:HB2	1:B:274:ASN:ND2	2.19	0.58
1:D:96:LEU:HD23	1:D:313:PHE:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:TYR:CE1	1:D:296:LEU:HD21	2.39	0.58
1:A:233:ILE:HG13	1:A:233:ILE:O	2.03	0.58
1:A:170:VAL:HG11	1:A:231:LYS:HB3	1.86	0.58
1:C:262:THR:O	1:C:266:THR:HG23	2.04	0.58
1:D:314:LYS:HB3	1:D:319:ILE:HB	1.86	0.58
1:D:185:ASN:HD22	1:D:187:LYS:H	1.52	0.57
1:D:241:PHE:HE1	1:D:245:MSE:SE	2.37	0.57
1:B:74:SER:O	1:B:153:ASP:HB2	2.04	0.57
1:C:147:MSE:HE3	1:C:309:VAL:HG23	1.85	0.57
1:A:314:LYS:HB3	1:A:319:ILE:HG23	1.84	0.57
1:B:173:ILE:CD1	1:B:228:ILE:HD13	2.35	0.57
1:B:185:ASN:HD22	1:B:187:LYS:H	1.51	0.57
1:D:78:MSE:HA	1:D:93:THR:O	2.05	0.57
1:D:240:ASN:O	1:D:244:ILE:CD1	2.53	0.57
1:C:182:THR:HG23	1:C:186:SER:HA	1.87	0.57
1:D:179:ILE:O	1:D:181:LEU:HG	2.04	0.56
1:D:118:ASP:OD1	1:D:119:TYR:HD1	1.87	0.56
1:A:96:LEU:HD13	1:A:97:ALA:N	2.21	0.56
1:C:75:VAL:HA	1:C:154:TYR:O	2.05	0.56
1:C:105:ALA:HB2	1:C:274:ASN:ND2	2.21	0.56
1:A:256:MSE:SE	1:A:264:MSE:HE1	2.55	0.56
1:B:98:THR:HG21	1:B:316:SER:OG	2.06	0.56
1:B:116:LYS:CG	1:B:124:ILE:HD11	2.27	0.56
1:B:159:ASN:ND2	1:B:159:ASN:C	2.57	0.56
1:B:256:MSE:HE3	1:B:264:MSE:HE3	1.87	0.56
1:C:161:GLU:OE1	1:C:164:LYS:NZ	2.30	0.56
1:A:147:MSE:HE2	1:A:310:ILE:HG13	1.87	0.56
1:C:257:THR:O	1:C:260:ASP:HB2	2.06	0.56
1:C:124:ILE:N	1:C:124:ILE:HD12	2.20	0.56
1:C:234:SER:C	1:C:236:SER:H	2.14	0.56
1:B:145:LYS:HB3	1:B:145:LYS:HZ3	1.71	0.56
1:A:222:ARG:HD2	1:A:277:SER:OG	2.06	0.55
1:A:242:GLU:C	1:A:244:ILE:H	2.14	0.55
1:D:319:ILE:HG12	1:D:320:THR:N	2.20	0.55
1:A:244:ILE:HG13	1:A:244:ILE:O	2.06	0.55
1:C:156:ILE:HD11	1:C:256:MSE:HE2	1.87	0.55
1:C:282:GLY:C	1:C:283:GLU:HG3	2.31	0.55
1:A:159:ASN:OD1	1:A:251:ASN:HB3	2.06	0.55
1:A:255:ASN:HD22	1:A:255:ASN:C	2.14	0.55
1:D:100:ASN:OD1	1:D:103:GLN:HG3	2.05	0.55
1:A:251:ASN:N	1:A:251:ASN:HD22	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLU:OE1	1:B:276:ASP:HB2	2.06	0.55
1:D:113:ARG:O	1:D:127:ILE:HG22	2.07	0.55
1:B:72:PRO:CB	1:B:100:ASN:HB2	2.31	0.55
1:B:265:ALA:O	1:B:269:SER:HB3	2.07	0.55
1:C:100:ASN:ND2	1:C:103:GLN:H	2.05	0.55
1:A:99:ALA:HB1	1:A:271:VAL:HG21	1.88	0.55
1:B:128:ASN:ND2	1:B:129:ALA:N	2.55	0.55
1:B:164:LYS:NZ	1:C:165:ASP:OD1	2.38	0.54
1:C:72:PRO:HG3	1:C:100:ASN:CG	2.33	0.54
1:A:77:LEU:HD23	1:A:156:ILE:CG2	2.38	0.54
1:A:319:ILE:HD13	1:A:319:ILE:N	2.22	0.54
1:C:269:SER:OG	1:D:176:TYR:HE1	1.91	0.54
1:A:149:GLY:HA3	1:A:314:LYS:CE	2.37	0.54
1:A:248:VAL:CG1	1:A:252:PHE:HB2	2.37	0.54
1:B:172:GLY:O	1:B:173:ILE:HD12	2.06	0.54
1:A:228:ILE:O	1:A:232:VAL:HG23	2.07	0.54
1:B:70:LYS:HD2	1:B:101:LYS:HG3	1.89	0.54
1:C:103:GLN:OE1	1:C:316:SER:HA	2.06	0.54
1:D:268:TYR:HB3	1:D:271:VAL:CG2	2.38	0.54
1:B:94:ILE:N	1:B:94:ILE:HD12	2.22	0.54
1:D:173:ILE:HD12	1:D:227:GLY:C	2.32	0.54
1:A:130:SER:OG	1:A:139:THR:HA	2.08	0.54
1:C:174:THR:OG1	1:C:194:THR:HG22	2.08	0.54
1:C:238:VAL:CG1	1:C:262:THR:HG23	2.38	0.54
1:C:110:SER:O	1:C:279:GLU:HG3	2.07	0.54
1:D:145:LYS:HB2	1:D:145:LYS:NZ	2.22	0.54
1:D:185:ASN:ND2	1:D:186:SER:N	2.48	0.54
1:C:256:MSE:SE	1:C:264:MSE:HE3	2.58	0.53
1:B:128:ASN:HD22	1:B:129:ALA:N	2.07	0.53
1:B:207:ARG:NH1	1:B:217:ARG:NH1	2.57	0.53
1:A:155:PHE:CD1	1:A:155:PHE:C	2.87	0.53
1:B:161:GLU:OE1	1:C:161:GLU:HB3	2.09	0.53
1:D:173:ILE:CD1	1:D:228:ILE:HA	2.37	0.53
1:D:158:ILE:HD13	1:D:158:ILE:N	2.24	0.52
1:A:160:MSE:HG3	1:A:205:ARG:NH2	2.22	0.52
1:B:256:MSE:HE2	1:B:261:ILE:HG12	1.91	0.52
1:C:154:TYR:HA	1:C:255:ASN:HD21	1.75	0.52
1:B:219:ASP:O	1:B:222:ARG:HB3	2.09	0.52
1:C:175:VAL:HG23	1:C:193:ILE:HD11	1.91	0.52
1:A:111:ILE:O	1:A:111:ILE:HG13	2.08	0.52
1:A:248:VAL:HG12	1:A:252:PHE:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ASN:HD22	1:D:270:SER:HB2	1.74	0.52
1:B:294:PHE:HD1	1:B:295:ASP:N	2.07	0.52
1:C:176:TYR:HE1	1:D:269:SER:OG	1.91	0.52
1:C:107:GLU:OE2	1:C:276:ASP:HB3	2.10	0.52
1:C:140:VAL:O	1:C:144:GLU:HB2	2.08	0.52
1:A:127:ILE:HD13	1:A:127:ILE:O	2.09	0.52
1:A:201:LEU:O	1:A:204:VAL:HG22	2.10	0.52
1:C:294:PHE:CD1	1:C:294:PHE:N	2.78	0.52
1:D:170:VAL:HG11	1:D:231:LYS:CB	2.40	0.51
1:D:217:ARG:HH22	2:D:322:PEG:H12	1.74	0.51
1:A:111:ILE:HD12	1:A:112:PRO:O	2.10	0.51
1:A:149:GLY:HA3	1:A:314:LYS:HE2	1.92	0.51
1:D:170:VAL:CG1	1:D:231:LYS:HB3	2.40	0.51
1:B:103:GLN:HE21	1:B:316:SER:HA	1.74	0.51
1:A:318:ASP:O	1:A:319:ILE:C	2.53	0.51
1:B:100:ASN:HD21	1:B:102:GLN:HB2	1.72	0.51
1:B:311:ASN:O	1:B:314:LYS:HB2	2.10	0.51
1:D:170:VAL:HG22	1:D:244:ILE:HG12	1.93	0.51
1:C:155:PHE:C	1:C:156:ILE:HD12	2.35	0.51
1:C:158:ILE:HG22	1:C:252:PHE:HA	1.93	0.51
1:C:306:LEU:O	1:C:309:VAL:HG22	2.11	0.51
1:C:165:ASP:HB2	1:C:248:VAL:HG12	1.93	0.51
1:A:180:ASP:HB2	1:A:190:LYS:CE	2.39	0.51
1:C:248:VAL:HG23	1:C:248:VAL:O	2.10	0.51
1:A:176:TYR:CE1	1:A:191:GLY:HA2	2.45	0.50
1:B:285:GLU:N	1:B:298:TYR:O	2.34	0.50
1:A:163:PHE:CZ	1:A:224:VAL:HG11	2.46	0.50
1:D:104:ASN:HD22	1:D:270:SER:CB	2.25	0.50
1:A:287:ILE:HD12	1:A:287:ILE:N	2.26	0.50
1:D:241:PHE:CD1	1:D:241:PHE:O	2.65	0.50
1:A:302:ASP:OD1	1:A:304:THR:HB	2.11	0.50
1:C:173:ILE:O	1:C:194:THR:HA	2.12	0.50
1:D:240:ASN:O	1:D:243:SER:HB3	2.11	0.50
1:B:154:TYR:HA	1:B:255:ASN:HD21	1.75	0.50
1:C:73:PHE:CE2	1:C:99:ALA:HB3	2.46	0.50
1:A:206:ILE:HG22	1:A:207:ARG:N	2.25	0.50
1:A:258:LEU:H	1:A:258:LEU:CD1	2.24	0.50
1:B:308:ARG:HG2	1:B:308:ARG:NH1	2.27	0.50
1:B:105:ALA:HB2	1:B:274:ASN:HD21	1.76	0.50
1:C:244:ILE:HG22	1:C:245:MSE:HE2	1.94	0.50
1:B:124:ILE:HG13	1:B:298:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:MSE:HE2	1:D:277:SER:HB2	1.94	0.49
1:C:125:GLY:CA	1:C:298:TYR:CE1	2.95	0.49
1:B:316:SER:C	1:B:317:LEU:HD12	2.37	0.49
1:B:103:GLN:NE2	1:B:316:SER:HA	2.27	0.49
1:B:117:VAL:HG13	1:B:117:VAL:O	2.12	0.49
1:C:98:THR:OG1	1:C:317:LEU:HD11	2.13	0.49
1:D:281:LYS:HA	1:D:281:LYS:CE	2.37	0.49
1:D:116:LYS:CG	1:D:124:ILE:HD11	2.42	0.49
1:D:163:PHE:CZ	1:D:224:VAL:HG11	2.44	0.49
1:A:102:GLN:H	1:A:102:GLN:CD	2.21	0.49
1:C:175:VAL:O	1:C:193:ILE:HD13	2.12	0.49
1:C:179:ILE:O	1:C:179:ILE:HG23	2.13	0.49
1:D:105:ALA:HA	1:D:274:ASN:O	2.13	0.49
1:D:158:ILE:HG22	1:D:252:PHE:HB2	1.94	0.49
1:C:228:ILE:O	1:C:232:VAL:HG23	2.12	0.48
1:B:182:THR:HG23	1:B:186:SER:HA	1.95	0.48
1:D:292:TYR:HB3	1:D:294:PHE:CE1	2.48	0.48
1:A:195:LEU:HD13	1:A:200:ALA:HA	1.94	0.48
1:C:313:PHE:O	1:C:317:LEU:HB2	2.13	0.48
1:D:241:PHE:HA	1:D:244:ILE:HD13	1.94	0.48
1:B:289:SER:CB	1:B:296:LEU:HD22	2.44	0.48
1:B:294:PHE:CD1	1:B:295:ASP:N	2.81	0.48
1:A:156:ILE:HD13	1:A:156:ILE:C	2.37	0.48
1:B:179:ILE:HG21	1:B:211:PRO:HD2	1.95	0.48
1:C:179:ILE:HA	1:C:190:LYS:HE3	1.94	0.48
1:C:155:PHE:C	1:C:155:PHE:CD1	2.91	0.48
1:D:170:VAL:HG11	1:D:231:LYS:HB3	1.95	0.48
1:A:257:THR:H	1:A:260:ASP:HB2	1.79	0.48
1:A:252:PHE:HE2	1:A:254:THR:CG2	2.27	0.48
1:B:98:THR:O	1:B:106:VAL:HA	2.13	0.48
1:C:315:LYS:C	1:C:317:LEU:N	2.72	0.48
1:D:75:VAL:O	1:D:75:VAL:HG13	2.13	0.48
1:D:154:TYR:HA	1:D:255:ASN:HD21	1.78	0.48
1:C:101:LYS:HE3	1:C:268:TYR:HA	1.94	0.48
1:D:118:ASP:OD1	1:D:119:TYR:CD1	2.66	0.48
1:B:146:LEU:C	1:B:147:MSE:HG3	2.38	0.47
1:C:158:ILE:HD11	2:C:322:PEG:H11	1.96	0.47
1:A:100:ASN:OD1	1:A:103:GLN:N	2.46	0.47
1:A:147:MSE:HA	1:A:310:ILE:HD11	1.95	0.47
1:B:90:ARG:HB2	1:B:128:ASN:O	2.15	0.47
1:C:100:ASN:ND2	1:C:103:GLN:HG3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:SER:HB3	1:D:176:TYR:OH	2.14	0.47
1:B:79:GLY:HA2	1:B:158:ILE:O	2.15	0.47
1:B:316:SER:O	1:B:317:LEU:HD12	2.15	0.47
1:A:224:VAL:O	1:A:228:ILE:HG13	2.15	0.47
1:C:279:GLU:O	1:C:280:LEU:C	2.56	0.47
1:A:242:GLU:CG	1:A:244:ILE:HG22	2.37	0.47
1:C:110:SER:OG	1:C:279:GLU:HB2	2.15	0.47
1:B:173:ILE:HD13	1:B:228:ILE:HD13	1.97	0.47
1:D:99:ALA:HB1	1:D:271:VAL:HG11	1.97	0.47
1:B:140:VAL:HA	1:B:143:VAL:HG12	1.96	0.46
1:A:183:GLU:OE2	1:A:183:GLU:HA	2.15	0.46
1:B:101:LYS:O	1:B:102:GLN:C	2.58	0.46
1:B:147:MSE:HB3	1:B:310:ILE:CG1	2.40	0.46
1:D:116:LYS:HG2	1:D:124:ILE:HD11	1.97	0.46
1:D:165:ASP:O	1:D:169:ALA:HB2	2.15	0.46
1:D:268:TYR:HB3	1:D:271:VAL:HG21	1.96	0.46
1:B:94:ILE:HB	1:B:111:ILE:HG12	1.98	0.46
1:D:76:LEU:CD2	1:D:78:MSE:HE2	2.42	0.46
1:A:251:ASN:N	1:A:251:ASN:ND2	2.64	0.46
1:B:248:VAL:HG12	1:B:252:PHE:HB2	1.97	0.46
1:C:111:ILE:HD13	1:C:280:LEU:HD22	1.97	0.46
1:D:255:ASN:H	1:D:255:ASN:HD22	1.62	0.46
1:A:159:ASN:HD21	1:A:161:GLU:HB2	1.77	0.46
1:D:95:ILE:HD12	1:D:95:ILE:N	2.30	0.46
1:B:246:LYS:HZ3	1:C:202:GLN:HE21	1.63	0.46
1:C:69:LYS:CG	1:C:70:LYS:H	2.27	0.46
1:B:121:ASN:OD1	1:B:121:ASN:C	2.58	0.46
1:C:181:LEU:HB2	1:C:188:PHE:HB3	1.98	0.46
1:D:145:LYS:HB2	1:D:145:LYS:HZ2	1.81	0.46
1:D:252:PHE:CD1	1:D:252:PHE:C	2.93	0.46
1:A:71:LYS:HG3	1:A:72:PRO:HD2	1.98	0.46
1:B:301:PRO:HD2	3:B:330:HOH:O	2.14	0.46
1:B:76:LEU:HD11	1:B:94:ILE:CG2	2.45	0.46
1:B:178:ASP:OD1	1:B:178:ASP:N	2.48	0.46
1:A:315:LYS:O	1:A:315:LYS:HD3	2.16	0.45
1:D:127:ILE:HD12	1:D:142:ALA:HB1	1.97	0.45
1:D:127:ILE:CD1	1:D:142:ALA:HB1	2.46	0.45
1:D:193:ILE:HD12	1:D:195:LEU:HD21	1.98	0.45
1:C:108:MSE:HE1	1:C:222:ARG:HG3	1.98	0.45
1:C:181:LEU:HD13	1:C:206:ILE:HD12	1.98	0.45
1:A:106:VAL:CG2	1:A:271:VAL:HG13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASN:C	1:A:255:ASN:ND2	2.74	0.45
1:B:128:ASN:HD22	1:B:128:ASN:C	2.25	0.45
1:C:69:LYS:HE3	1:C:71:LYS:HG3	1.99	0.45
1:C:218:GLN:HE21	1:C:221:GLN:NE2	2.14	0.45
1:B:131:TYR:CE1	1:B:136:PRO:HG3	2.52	0.45
1:D:149:GLY:HA3	1:D:314:LYS:HE2	1.98	0.45
1:B:170:VAL:HG22	1:B:231:LYS:HB3	1.99	0.45
1:B:93:THR:C	1:B:94:ILE:HD12	2.42	0.45
1:C:127:ILE:C	1:C:129:ALA:N	2.73	0.45
1:D:185:ASN:ND2	1:D:187:LYS:HG3	2.31	0.45
1:B:155:PHE:CD1	1:B:155:PHE:C	2.94	0.45
1:C:282:GLY:O	1:C:283:GLU:HG3	2.17	0.45
1:A:90:ARG:HH11	1:A:90:ARG:HG3	1.82	0.45
1:B:115:THR:HG23	1:B:301:PRO:HG3	1.97	0.45
1:D:111:ILE:HD12	1:D:146:LEU:CD2	2.47	0.45
1:C:104:ASN:O	1:C:274:ASN:ND2	2.49	0.45
1:D:128:ASN:OD1	1:D:128:ASN:C	2.60	0.45
1:D:255:ASN:HD22	1:D:255:ASN:C	2.24	0.45
1:B:97:ALA:HA	1:B:107:GLU:O	2.17	0.44
1:C:317:LEU:HB3	1:C:318:ASP:H	1.64	0.44
1:D:226:ILE:HD11	1:D:275:VAL:HG21	1.98	0.44
1:A:77:LEU:HB2	1:A:95:ILE:HB	1.99	0.44
1:B:256:MSE:HE2	1:B:261:ILE:CG1	2.46	0.44
1:A:156:ILE:O	1:A:156:ILE:HG23	2.18	0.44
1:A:252:PHE:HE2	1:A:254:THR:HG21	1.82	0.44
1:B:194:THR:C	1:B:195:LEU:HD23	2.41	0.44
1:C:229:ALA:HB1	1:C:272:LEU:HD21	2.00	0.44
1:D:292:TYR:HB3	1:D:294:PHE:CZ	2.52	0.44
1:A:108:MSE:O	1:A:277:SER:HA	2.18	0.44
1:D:156:ILE:HG12	1:D:256:MSE:HE2	1.99	0.44
1:D:201:LEU:O	1:D:204:VAL:HG22	2.17	0.44
1:B:111:ILE:O	1:B:111:ILE:HG13	2.17	0.44
1:B:302:ASP:OD1	1:B:302:ASP:C	2.61	0.44
1:C:113:ARG:HB2	1:C:128:ASN:CB	2.47	0.44
1:D:159:ASN:HD21	1:D:251:ASN:HA	1.82	0.44
1:D:180:ASP:OD2	1:D:180:ASP:C	2.60	0.44
1:A:158:ILE:HD12	1:A:158:ILE:C	2.43	0.43
1:B:124:ILE:HD12	1:B:125:GLY:N	2.33	0.43
1:C:76:LEU:HD12	1:C:95:ILE:O	2.18	0.43
1:C:90:ARG:HG3	1:C:90:ARG:HH11	1.82	0.43
1:C:232:VAL:O	1:C:232:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ARG:HG3	1:D:128:ASN:CB	2.45	0.43
1:A:269:SER:OG	1:B:176:TYR:HE1	2.02	0.43
1:C:310:ILE:O	1:C:314:LYS:HG3	2.18	0.43
1:D:112:PRO:HG3	1:D:279:GLU:OE1	2.18	0.43
1:D:255:ASN:C	1:D:255:ASN:ND2	2.77	0.43
1:C:111:ILE:HA	1:C:280:LEU:CD2	2.44	0.43
1:D:76:LEU:C	1:D:77:LEU:HD12	2.43	0.43
1:D:111:ILE:HG12	1:D:111:ILE:O	2.17	0.43
1:D:130:SER:OG	1:D:139:THR:HA	2.18	0.43
1:A:167:VAL:HG13	1:A:173:ILE:HG23	2.00	0.43
1:D:78:MSE:O	1:D:158:ILE:HD13	2.18	0.43
1:D:188:PHE:N	1:D:188:PHE:CD1	2.86	0.43
1:D:315:LYS:HB2	1:D:315:LYS:HE3	1.65	0.43
1:B:81:ASP:HA	1:B:159:ASN:HB2	2.00	0.43
1:B:131:TYR:HE1	1:B:136:PRO:HG3	1.82	0.43
1:D:219:ASP:C	1:D:219:ASP:OD1	2.61	0.43
1:B:78:MSE:HA	1:B:93:THR:O	2.19	0.43
1:B:100:ASN:O	1:B:104:ASN:HA	2.19	0.43
1:C:156:ILE:HD12	1:C:156:ILE:N	2.34	0.43
1:D:91:ALA:HB2	1:D:131:TYR:HB2	2.01	0.43
1:A:124:ILE:N	1:A:124:ILE:CD1	2.73	0.43
1:A:140:VAL:O	1:A:144:GLU:HG3	2.19	0.43
1:B:111:ILE:O	1:B:111:ILE:CG1	2.66	0.43
1:B:228:ILE:O	1:B:232:VAL:HG23	2.18	0.43
1:B:266:THR:O	1:B:266:THR:HG22	2.19	0.42
1:A:269:SER:OG	1:B:176:TYR:CE1	2.71	0.42
1:C:98:THR:HG21	1:C:316:SER:HB3	2.02	0.42
1:C:181:LEU:O	1:C:183:GLU:N	2.48	0.42
1:A:201:LEU:HA	1:A:204:VAL:HG22	2.01	0.42
1:C:177:ASN:HB2	1:C:193:ILE:HD12	2.02	0.42
1:C:210:ASP:C	1:C:212:ARG:H	2.28	0.42
1:D:265:ALA:O	1:D:269:SER:HB2	2.20	0.42
1:A:184:VAL:HG11	1:A:206:ILE:CD1	2.41	0.42
1:B:286:MSE:C	1:B:287:ILE:HG13	2.44	0.42
1:B:185:ASN:C	1:B:185:ASN:ND2	2.69	0.42
1:B:253:GLN:N	1:B:253:GLN:OE1	2.53	0.42
1:C:94:ILE:O	1:C:110:SER:HA	2.20	0.42
1:A:165:ASP:O	1:A:168:ASP:N	2.53	0.42
1:A:200:ALA:O	1:A:204:VAL:HG13	2.19	0.42
1:A:204:VAL:CG1	1:A:224:VAL:HG21	2.50	0.42
1:B:234:SER:O	1:B:236:SER:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:GLN:O	1:C:225:ILE:HG13	2.19	0.42
1:C:222:ARG:HH21	1:C:275:VAL:HG13	1.84	0.42
1:C:125:GLY:HA3	1:C:298:TYR:CE1	2.53	0.42
1:D:102:GLN:N	1:D:102:GLN:OE1	2.53	0.42
1:D:168:ASP:OD1	1:D:196:ASN:HB2	2.20	0.42
1:C:108:MSE:CE	1:C:222:ARG:HG3	2.50	0.42
1:D:111:ILE:O	1:D:111:ILE:CG1	2.67	0.42
1:D:173:ILE:O	1:D:194:THR:HA	2.19	0.42
1:D:222:ARG:O	1:D:226:ILE:HG12	2.20	0.42
1:A:166:LEU:CD1	1:A:244:ILE:HD11	2.49	0.42
1:B:282:GLY:HA3	1:B:300:ALA:O	2.20	0.42
1:C:77:LEU:HD12	1:C:156:ILE:HB	2.02	0.42
1:C:268:TYR:O	1:C:269:SER:C	2.63	0.42
1:D:77:LEU:HD12	1:D:77:LEU:N	2.35	0.42
1:B:90:ARG:NH1	1:B:90:ARG:HG2	2.35	0.41
1:B:167:VAL:HG22	1:B:228:ILE:CD1	2.47	0.41
1:C:195:LEU:HD22	1:C:199:ASP:HB3	2.02	0.41
1:C:270:SER:O	1:C:273:LYS:HB2	2.20	0.41
1:A:100:ASN:O	1:A:104:ASN:N	2.53	0.41
1:A:185:ASN:HB2	1:A:202:GLN:OE1	2.20	0.41
1:C:124:ILE:HG22	1:C:124:ILE:O	2.18	0.41
1:C:130:SER:OG	1:C:139:THR:HA	2.20	0.41
1:A:302:ASP:OD1	1:A:304:THR:N	2.54	0.41
1:B:159:ASN:ND2	1:B:162:GLY:N	2.55	0.41
1:B:182:THR:O	1:B:183:GLU:C	2.62	0.41
1:B:287:ILE:O	1:B:288:TYR:C	2.63	0.41
1:D:243:SER:HA	1:D:246:LYS:CE	2.49	0.41
1:B:289:SER:HB2	1:B:296:LEU:HD22	2.01	0.41
1:B:311:ASN:HA	1:B:314:LYS:HD2	2.02	0.41
1:A:242:GLU:C	1:A:244:ILE:N	2.79	0.41
1:B:160:MSE:HG3	1:B:205:ARG:HH21	1.83	0.41
1:B:224:VAL:O	1:B:228:ILE:HG12	2.21	0.41
1:C:156:ILE:CG1	1:C:256:MSE:HE2	2.50	0.41
1:B:273:LYS:HE2	1:B:273:LYS:HB3	1.85	0.41
1:B:306:LEU:O	1:B:310:ILE:CD1	2.58	0.41
1:D:243:SER:HA	1:D:246:LYS:HE3	2.03	0.41
1:C:170:VAL:O	1:C:170:VAL:HG13	2.19	0.41
1:A:108:MSE:HE2	1:A:275:VAL:HG12	1.97	0.41
1:D:319:ILE:CG1	1:D:320:THR:N	2.84	0.41
1:A:104:ASN:HD21	1:A:270:SER:CB	2.30	0.41
1:A:176:TYR:HE1	1:A:191:GLY:HA2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:CG2	1:A:207:ARG:N	2.84	0.41
1:A:308:ARG:HG2	1:A:308:ARG:HH11	1.86	0.41
1:D:155:PHE:CD1	1:D:155:PHE:C	2.98	0.41
1:D:204:VAL:HG11	1:D:224:VAL:HG21	2.03	0.41
1:A:200:ALA:O	1:A:203:TYR:HB3	2.21	0.41
1:C:156:ILE:HD11	1:C:256:MSE:CE	2.51	0.41
1:D:231:LYS:C	1:D:233:ILE:N	2.76	0.41
1:D:262:THR:O	1:D:266:THR:HG23	2.20	0.41
1:C:125:GLY:HA2	1:C:298:TYR:CE1	2.57	0.40
1:C:319:ILE:C	1:C:319:ILE:CD1	2.94	0.40
1:B:268:TYR:O	1:B:269:SER:C	2.64	0.40
1:D:164:LYS:HD2	1:D:198:THR:HA	2.04	0.40
1:D:173:ILE:HG22	1:D:175:VAL:HG13	2.03	0.40
1:B:101:LYS:O	1:B:104:ASN:N	2.55	0.40
1:B:140:VAL:C	1:B:143:VAL:HG12	2.46	0.40
1:B:312:MSE:C	1:B:314:LYS:N	2.79	0.40
1:C:109:VAL:HG23	1:C:313:PHE:CZ	2.56	0.40
1:A:76:LEU:HD13	1:A:96:LEU:HD23	2.03	0.40
1:B:90:ARG:HA	1:B:131:TYR:HB3	2.03	0.40
1:B:100:ASN:ND2	1:B:103:GLN:OE1	2.43	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	229/321 (71%)	200 (87%)	24 (10%)	5 (2%)	5	10
1	B	225/321 (70%)	192 (85%)	27 (12%)	6 (3%)	4	7
1	C	231/321 (72%)	199 (86%)	29 (13%)	3 (1%)	9	21
1	D	229/321 (71%)	208 (91%)	18 (8%)	3 (1%)	9	21
All	All	914/1284 (71%)	799 (87%)	98 (11%)	17 (2%)	6	13

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	SER
1	B	102	GLN
1	B	235	SER
1	C	269	SER
1	A	166	LEU
1	B	180	ASP
1	D	269	SER
1	A	102	GLN
1	B	80	SER
1	D	188	PHE
1	A	319	ILE
1	B	269	SER
1	B	89	GLY
1	C	148	PRO
1	A	189	VAL
1	D	148	PRO
1	C	237	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	205/269 (76%)	184 (90%)	21 (10%)	7	15
1	B	200/269 (74%)	179 (90%)	21 (10%)	6	14
1	C	206/269 (77%)	187 (91%)	19 (9%)	8	19
1	D	206/269 (77%)	187 (91%)	19 (9%)	8	19
All	All	817/1076 (76%)	737 (90%)	80 (10%)	7	17

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	102	GLN
1	A	107	GLU

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Mol	Chain	Res	Type
1	A	111	ILE
1	A	117	VAL
1	A	124	ILE
1	A	127	ILE
1	A	156	ILE
1	A	174	THR
1	A	178	ASP
1	A	181	LEU
1	A	219	ASP
1	A	244	ILE
1	A	254	THR
1	A	255	ASN
1	A	258	LEU
1	A	271	VAL
1	A	296	LEU
1	A	310	ILE
1	A	315	LYS
1	A	319	ILE
1	B	71	LYS
1	B	90	ARG
1	B	96	LEU
1	B	98	THR
1	B	113	ARG
1	B	121	ASN
1	B	127	ILE
1	B	128	ASN
1	B	158	ILE
1	B	159	ASN
1	B	173	ILE
1	B	178	ASP
1	B	185	ASN
1	B	218	GLN
1	B	245	MSE
1	B	257	THR
1	B	258	LEU
1	B	272	LEU
1	B	275	VAL
1	B	296	LEU
1	B	302	ASP
1	C	75	VAL
1	C	77	LEU
1	C	98	THR

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Mol	Chain	Res	Type
1	C	101	LYS
1	C	104	ASN
1	C	113	ARG
1	C	128	ASN
1	C	170	VAL
1	C	173	ILE
1	C	183	GLU
1	C	193	ILE
1	C	242	GLU
1	C	271	VAL
1	C	272	LEU
1	C	274	ASN
1	C	294	PHE
1	C	306	LEU
1	C	317	LEU
1	C	319	ILE
1	D	78	MSE
1	D	102	GLN
1	D	111	ILE
1	D	145	LYS
1	D	148	PRO
1	D	158	ILE
1	D	185	ASN
1	D	190	LYS
1	D	219	ASP
1	D	252	PHE
1	D	255	ASN
1	D	258	LEU
1	D	280	LEU
1	D	289	SER
1	D	296	LEU
1	D	304	THR
1	D	306	LEU
1	D	309	VAL
1	D	318	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	104	ASN
1	A	230	ASN

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Mol	Chain	Res	Type
1	A	251	ASN
1	A	255	ASN
1	B	100	ASN
1	B	128	ASN
1	B	159	ASN
1	B	185	ASN
1	B	230	ASN
1	B	267	ASN
1	B	274	ASN
1	B	311	ASN
1	C	100	ASN
1	C	104	ASN
1	C	159	ASN
1	C	202	GLN
1	C	218	GLN
1	C	221	GLN
1	D	104	ASN
1	D	185	ASN
1	D	221	GLN
1	D	251	ASN
1	D	255	ASN
1	D	278	GLN
1	D	311	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEG	C	322	-	6,6,6	0.48	0	5,5,5	0.71	0
2	PEG	D	322	-	6,6,6	0.56	0	5,5,5	0.64	0
2	PEG	B	322	-	6,6,6	0.59	0	5,5,5	0.68	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
2	PEG	C	322	-	-	1/4/4/4	-
2	PEG	D	322	-	-	1/4/4/4	-
2	PEG	B	322	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	322	PEG	O2-C3-C4-O4
2	B	322	PEG	O1-C1-C2-O2
2	C	322	PEG	O2-C3-C4-O4
2	D	322	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	322	PEG	1	0
2	D	322	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	228/321 (71%)	0.17	6 (2%) 57 51	31, 52, 82, 122	0
1	B	224/321 (69%)	0.22	6 (2%) 56 50	22, 56, 84, 110	0
1	C	228/321 (71%)	0.20	4 (1%) 67 63	23, 53, 87, 134	0
1	D	228/321 (71%)	0.13	7 (3%) 51 45	28, 51, 77, 120	0
All	All	908/1284 (70%)	0.18	23 (2%) 58 52	22, 53, 84, 134	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	ILE	4.3
1	C	238	VAL	3.6
1	D	320	THR	3.4
1	D	240	ASN	3.2
1	D	215	PHE	3.2
1	C	182	THR	3.0
1	A	234	SER	2.8
1	C	235	SER	2.8
1	B	318	ASP	2.8
1	C	241	PHE	2.8
1	D	89	GLY	2.6
1	B	154	TYR	2.5
1	A	81	ASP	2.4
1	A	320	THR	2.4
1	B	124	ILE	2.2
1	B	294	PHE	2.2
1	B	81	ASP	2.2
1	D	319	ILE	2.2
1	B	121	ASN	2.1
1	A	258	LEU	2.1
1	A	208	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	81	ASP	2.0
1	D	133	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	PEG	D	322	7/7	0.79	0.15	49,63,72,75	0
2	PEG	C	322	7/7	0.87	0.11	46,54,61,62	0
2	PEG	B	322	7/7	0.89	0.09	58,63,71,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.