



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:01 PM UTC

PDB ID : 3K92 / pdb_00003k92
Title : Crystal structure of a E93K mutant of the major Bacillus subtilis glutamate dehydrogenase RocG
Authors : Gunka, K.; Newman, J.A.; Commichau, F.M.; Herzberg, C.; Rodrigues, C.; Hewitt, L.; Lewis, R.J.; Stulke, J.
Deposited on : 2009-10-15
Resolution : 2.30 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

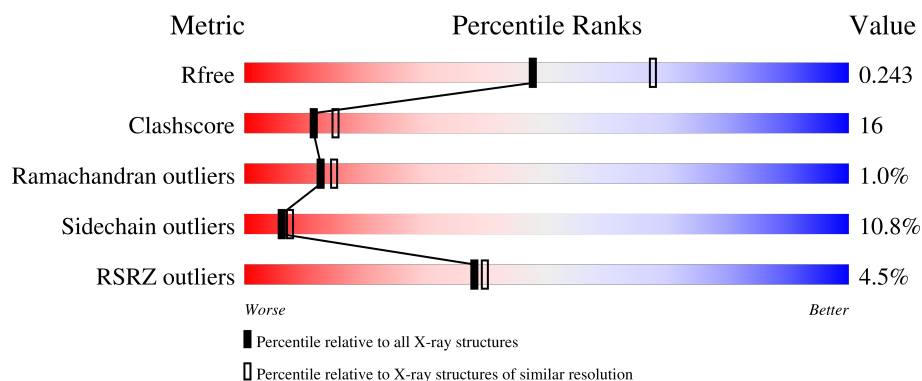
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	424	8% 72% 20% 5% ..
1	B	424	69% 21% 5% ..
1	C	424	8% 66% 24% 6% .
1	D	424	2% 69% 21% 5% .
1	E	424	9% 59% 27% 6% . 7%

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Mol	Chain	Length	Quality of chain
1	F	424	

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
2	PEG	D	425	-	-	X	-
2	PEG	E	425	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19628 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.

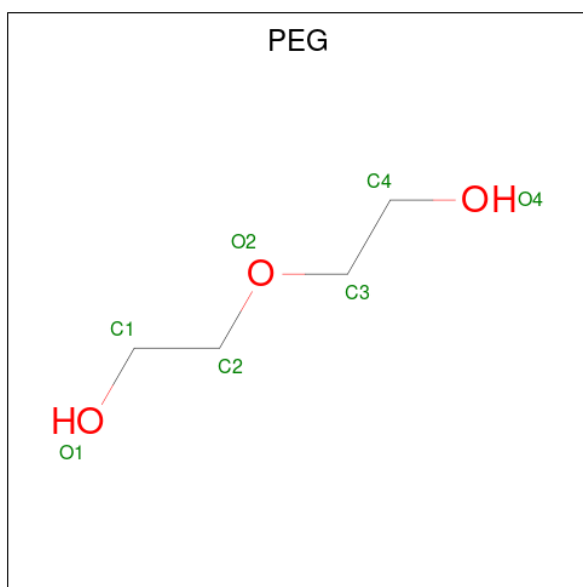
- Molecule 1 is a protein called NAD-specific glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3230	2042	556	614	18			
1	B	409	Total	C	N	O	S	0	0	0
			3158	1999	545	596	18			
1	C	409	Total	C	N	O	S	0	0	0
			3158	1999	545	596	18			
1	D	406	Total	C	N	O	S	0	0	0
			3129	1980	542	590	17			
1	E	396	Total	C	N	O	S	0	0	0
			3051	1932	528	574	17			
1	F	395	Total	C	N	O	S	0	0	0
			3043	1928	526	572	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	LYS	GLU	engineered mutation	UNP P39633
A	324	ARG	ALA	SEE REMARK 999	UNP P39633
B	93	LYS	GLU	engineered mutation	UNP P39633
B	324	ARG	ALA	SEE REMARK 999	UNP P39633
C	93	LYS	GLU	engineered mutation	UNP P39633
C	324	ARG	ALA	SEE REMARK 999	UNP P39633
D	93	LYS	GLU	engineered mutation	UNP P39633
D	324	ARG	ALA	SEE REMARK 999	UNP P39633
E	93	LYS	GLU	engineered mutation	UNP P39633
E	324	ARG	ALA	SEE REMARK 999	UNP P39633
F	93	LYS	GLU	engineered mutation	UNP P39633
F	324	ARG	ALA	SEE REMARK 999	UNP P39633

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



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

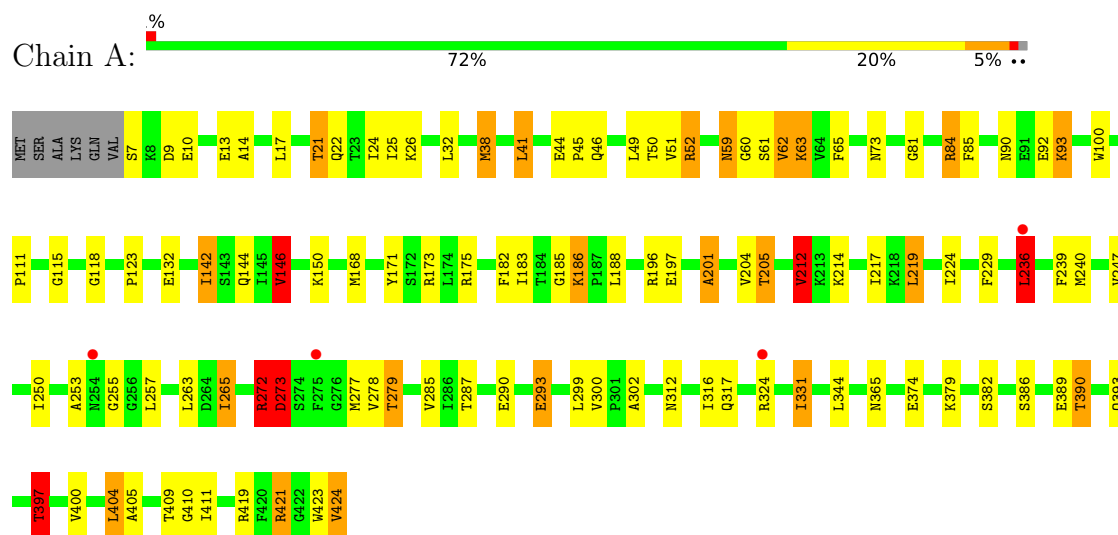
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	187	Total	O	0	0
			187	187		
3	B	161	Total	O	0	0
			161	161		
3	C	133	Total	O	0	0
			133	133		
3	D	112	Total	O	0	0
			112	112		
3	E	108	Total	O	0	0
			108	108		
3	F	123	Total	O	0	0
			123	123		

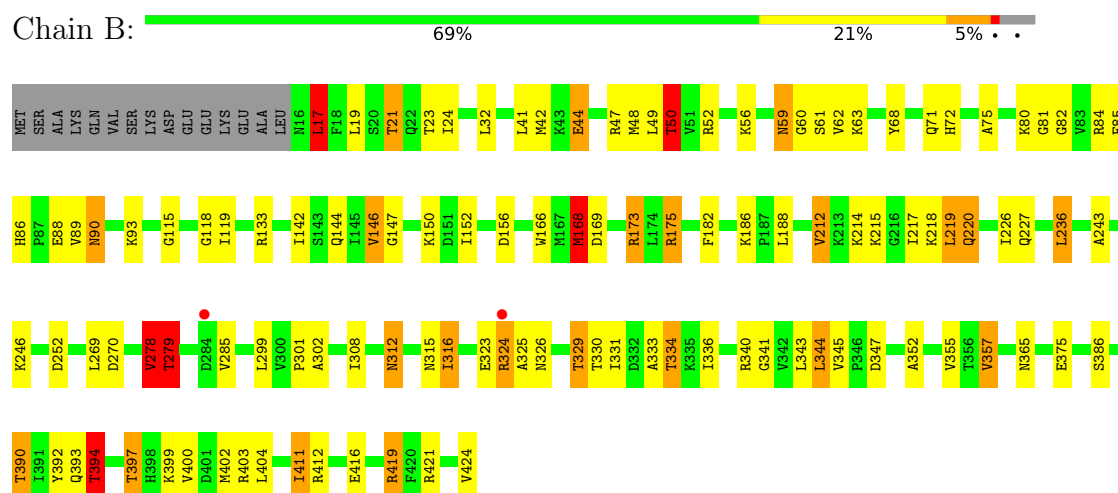
3 Residue-property plots

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: NAD-specific glutamate dehydrogenase

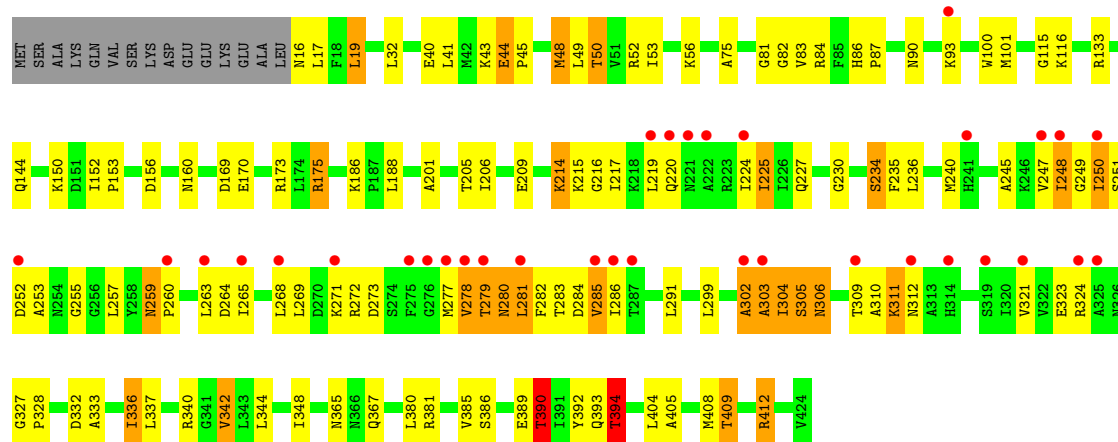


• Molecule 1: NAD-specific glutamate dehydrogenase

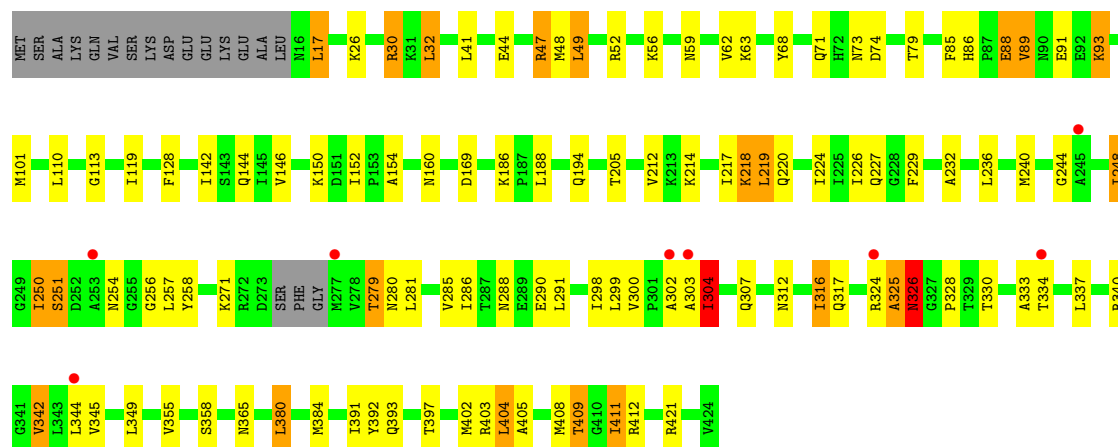


• Molecule 1: NAD-specific glutamate dehydrogenase

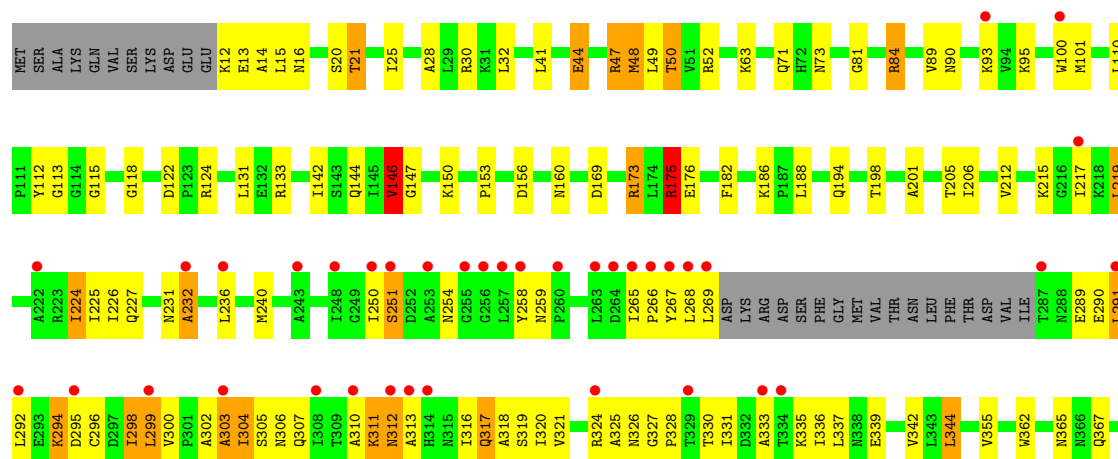




• Molecule 1: NAD-specific glutamate dehydrogenase

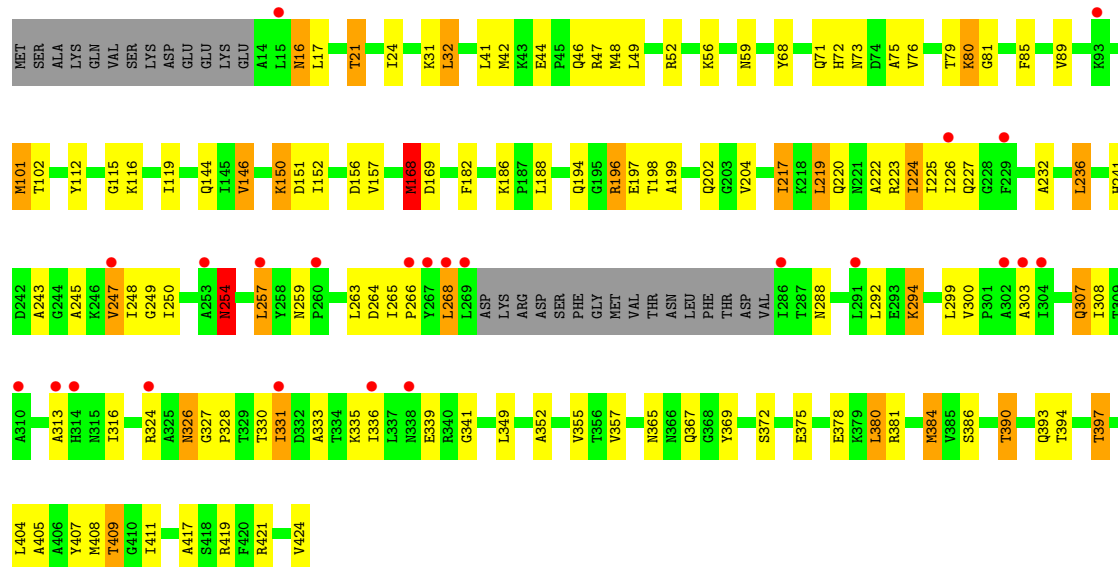


• Molecule 1: NAD-specific glutamate dehydrogenase





• Molecule 1: NAD-specific glutamate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.61Å 143.07Å 162.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.67 – 2.30 18.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (18.67-2.30) 99.6 (18.67-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.238 (Not available) , 0.243	Depositor DCC
R_{free} test set	7159 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19628	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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	1.37	9/3289 (0.3%)	1.24	12/4443 (0.3%)
1	B	1.34	10/3217 (0.3%)	1.24	18/4348 (0.4%)
1	C	1.27	7/3217 (0.2%)	1.13	6/4348 (0.1%)
1	D	1.22	7/3186 (0.2%)	1.15	6/4306 (0.1%)
1	E	1.25	5/3107 (0.2%)	1.19	13/4197 (0.3%)
1	F	1.27	9/3099 (0.3%)	1.16	7/4188 (0.2%)
All	All	1.29	47/19115 (0.2%)	1.19	62/25830 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	89	VAL	CA-CB	9.32	1.63	1.54
1	A	331	ILE	CA-CB	7.85	1.63	1.54
1	F	44	GLU	CA-C	7.31	1.59	1.52
1	A	146	VAL	CA-C	6.92	1.60	1.52
1	B	75	ALA	CA-CB	6.87	1.64	1.53
1	F	75	ALA	CA-CB	6.80	1.64	1.53
1	A	421	ARG	CD-NE	-6.65	1.36	1.46
1	B	44	GLU	CA-C	6.61	1.59	1.52
1	B	278	VAL	CA-CB	6.50	1.63	1.54
1	B	411	ILE	CA-CB	6.35	1.62	1.54
1	F	152	ILE	C-O	6.27	1.31	1.24
1	F	394	THR	CA-CB	6.27	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	PRO	CA-C	6.16	1.59	1.53
1	C	152	ILE	CA-C	5.93	1.59	1.52
1	C	390	THR	CA-CB	5.89	1.63	1.53
1	F	150	LYS	CA-C	5.84	1.58	1.52
1	A	183	ILE	CA-CB	5.77	1.62	1.54
1	D	154	ALA	CA-CB	5.75	1.62	1.53
1	C	53	ILE	CA-CB	5.67	1.61	1.54
1	A	52	ARG	CD-NE	-5.65	1.38	1.46
1	C	45	PRO	C-O	5.65	1.30	1.23
1	F	76	VAL	CA-CB	5.64	1.61	1.54
1	D	316	ILE	CA-CB	5.61	1.60	1.54
1	B	278	VAL	CA-C	5.60	1.59	1.52
1	B	63	LYS	CE-NZ	5.55	1.66	1.49
1	B	279	THR	CA-CB	5.54	1.62	1.53
1	D	411	ILE	CA-CB	5.54	1.62	1.54
1	E	44	GLU	CA-C	5.51	1.58	1.52
1	D	47	ARG	C-O	5.44	1.29	1.23
1	A	142	ILE	CA-CB	5.41	1.60	1.54
1	E	21	THR	CA-CB	5.38	1.61	1.53
1	B	394	THR	CA-CB	5.36	1.62	1.53
1	C	394	THR	CA-CB	5.33	1.61	1.53
1	A	51	VAL	CA-C	5.30	1.59	1.52
1	B	142	ILE	N-CA	5.27	1.53	1.46
1	D	89	VAL	CA-CB	5.17	1.59	1.54
1	B	168	MET	N-CA	-5.15	1.40	1.46
1	C	385	VAL	CA-CB	5.13	1.60	1.54
1	D	152	ILE	CA-C	5.13	1.58	1.52
1	A	201	ALA	C-O	-5.12	1.18	1.24
1	E	142	ILE	CA-CB	5.12	1.60	1.54
1	E	421	ARG	CD-NE	-5.09	1.39	1.46
1	D	152	ILE	CA-CB	-5.05	1.49	1.54
1	F	417	ALA	CA-CB	5.04	1.61	1.53
1	C	75	ALA	C-O	-5.03	1.18	1.24
1	E	331	ILE	CA-CB	5.03	1.60	1.54
1	F	196	ARG	CZ-NH1	5.00	1.39	1.32

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ARG	NE-CZ-NH2	-8.97	111.12	119.20
1	D	312	ASN	N-CA-C	7.68	119.65	111.28
1	E	47	ARG	NE-CZ-NH2	-6.87	113.01	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	VAL	N-CA-CB	-6.83	100.96	112.44
1	C	44	GLU	CA-C-N	-6.66	113.08	120.14
1	C	44	GLU	C-N-CA	-6.66	113.08	120.14
1	E	133	ARG	NE-CZ-NH2	-6.56	113.30	119.20
1	C	133	ARG	NE-CZ-NH2	-6.54	113.32	119.20
1	B	175	ARG	NE-CZ-NH1	6.49	127.98	121.50
1	A	52	ARG	NE-CZ-NH2	-6.45	113.39	119.20
1	A	236	LEU	N-CA-C	6.34	118.20	111.28
1	B	175	ARG	NE-CZ-NH2	-6.34	113.50	119.20
1	B	133	ARG	CG-CD-NE	-6.32	98.09	112.00
1	A	410	GLY	N-CA-C	6.23	120.74	112.77
1	E	224	ILE	N-CA-C	6.19	117.51	108.53
1	C	101	MET	CG-SD-CE	-6.14	87.39	100.90
1	F	254	ASN	N-CA-C	6.01	117.92	111.36
1	E	411	ILE	CB-CA-C	-5.99	102.08	110.95
1	B	44	GLU	CA-CB-CG	5.96	126.02	114.10
1	A	146	VAL	CG1-CB-CG2	5.95	123.89	110.80
1	B	175	ARG	CD-NE-CZ	5.95	132.72	124.40
1	E	133	ARG	CG-CD-NE	-5.87	99.09	112.00
1	B	82	GLY	N-CA-C	5.75	119.96	112.25
1	E	298	ILE	N-CA-C	5.68	116.30	108.12
1	A	272	ARG	N-CA-C	5.66	118.45	109.96
1	A	212	VAL	N-CA-C	-5.65	103.87	111.44
1	B	324	ARG	CB-CA-C	-5.60	102.27	110.95
1	F	326	ASN	N-CA-C	5.53	118.26	109.24
1	E	415	ALA	N-CA-C	-5.52	105.18	111.14
1	B	17	LEU	N-CA-C	-5.49	104.69	111.33
1	B	357	VAL	CB-CA-C	-5.46	103.41	112.26
1	B	44	GLU	N-CA-CB	-5.43	101.41	111.19
1	E	175	ARG	CD-NE-CZ	5.43	132.00	124.40
1	E	424	VAL	CB-CA-C	-5.40	101.13	111.40
1	F	168	MET	CG-SD-CE	5.39	112.75	100.90
1	A	397	THR	N-CA-CB	5.38	118.13	110.16
1	A	273	ASP	CB-CA-C	-5.37	99.73	110.42
1	E	175	ARG	NE-CZ-NH2	-5.37	114.37	119.20
1	C	170	GLU	N-CA-C	-5.36	105.51	111.36
1	A	186	LYS	CA-C-N	5.36	125.28	119.76
1	A	186	LYS	C-N-CA	5.36	125.28	119.76
1	F	424	VAL	CB-CA-C	-5.35	101.24	111.40
1	E	147	GLY	CA-C-N	5.31	124.97	119.56
1	E	147	GLY	C-N-CA	5.31	124.97	119.56
1	F	101	MET	CG-SD-CE	-5.29	89.26	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	THR	CB-CA-C	5.27	119.36	109.71
1	B	326	ASN	N-CA-C	5.26	118.97	112.24
1	E	146	VAL	N-CA-CB	-5.26	102.63	112.36
1	B	142	ILE	N-CA-C	5.26	117.95	112.90
1	D	254	ASN	N-CA-C	5.26	117.92	111.82
1	B	166	TRP	N-CA-C	5.20	116.95	111.28
1	D	312	ASN	CB-CA-C	-5.18	102.19	110.79
1	C	412	ARG	CG-CD-NE	-5.17	100.64	112.00
1	B	147	GLY	CA-C-N	5.16	125.46	119.47
1	B	147	GLY	C-N-CA	5.16	125.46	119.47
1	D	326	ASN	N-CA-C	5.14	121.75	110.80
1	D	128	PHE	CA-C-N	5.13	125.64	119.94
1	D	128	PHE	C-N-CA	5.13	125.64	119.94
1	F	16	ASN	N-CA-C	-5.06	104.28	110.65
1	B	357	VAL	N-CA-CB	5.04	119.90	110.77
1	F	341	GLY	N-CA-C	5.02	122.03	115.40
1	A	146	VAL	CB-CA-C	5.01	118.16	110.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	325	ALA	Peptide

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	3230	0	3248	106	0
1	B	3158	0	3179	97	0
1	C	3158	0	3179	111	0
1	D	3129	0	3145	100	0
1	E	3051	0	3075	124	0
1	F	3043	0	3072	103	0
2	A	7	0	10	0	0
2	C	7	0	10	3	0
2	D	7	0	10	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	7	0	10	4	0
2	F	7	0	10	0	0
3	A	187	0	0	6	0
3	B	161	0	0	11	0
3	C	133	0	0	7	0
3	D	112	0	0	4	0
3	E	108	0	0	6	0
3	F	123	0	0	8	0
All	All	19628	0	18948	609	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 16.

All (609) 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:E:295:ASP:HA	1:E:317:GLN:HE21	1.07	1.16
1:B:17:LEU:O	1:B:21:THR:HG23	1.59	1.02
1:E:14:ALA:HB2	1:E:93:LYS:HE3	1.45	0.96
1:A:205:THR:HG22	1:A:236:LEU:CD2	1.96	0.95
1:E:295:ASP:CA	1:E:317:GLN:HE21	1.79	0.95
1:C:16:ASN:N	1:C:19:LEU:HD23	1.81	0.95
1:C:90:ASN:HD21	1:C:93:LYS:HE3	1.32	0.95
1:A:38:MET:HE3	1:A:38:MET:HA	1.48	0.93
1:A:205:THR:HG22	1:A:236:LEU:HD21	1.50	0.93
1:A:405:ALA:O	1:A:409:THR:HG23	1.68	0.92
1:E:310:ALA:HB3	1:E:311:LYS:CE	2.01	0.91
1:D:325:ALA:HB1	1:D:326:ASN:HB2	1.52	0.90
1:F:386:SER:O	1:F:390:THR:HG23	1.71	0.90
1:F:250:ILE:HD13	1:F:263:LEU:HD22	1.51	0.90
1:E:333:ALA:O	1:E:337:LEU:HD13	1.72	0.89
1:E:312:ASN:O	1:E:316:ILE:HD12	1.72	0.89
1:E:295:ASP:HA	1:E:317:GLN:NE2	1.87	0.89
1:A:236:LEU:HD22	1:A:324:ARG:NH2	1.86	0.89
1:E:295:ASP:CA	1:E:317:GLN:NE2	2.36	0.88
1:C:215:LYS:O	1:C:217:ILE:HD12	1.73	0.87
1:E:90:ASN:ND2	1:E:93:LYS:HD2	1.89	0.87
1:C:16:ASN:N	1:C:19:LEU:CD2	2.39	0.86
1:A:150:LYS:NZ	1:B:144:GLN:HE21	1.73	0.86
1:C:268:LEU:HD23	1:C:278:VAL:HG11	1.57	0.85
1:F:219:LEU:HD13	1:F:243:ALA:HB1	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:MET:HE2	1:D:91:GLU:HG3	1.57	0.84
1:A:300:VAL:HG11	1:A:324:ARG:NE	1.93	0.83
1:E:310:ALA:HB3	1:E:311:LYS:HE3	1.61	0.83
1:A:201:ALA:O	1:A:205:THR:HG23	1.78	0.82
1:D:160:ASN:HD21	2:D:425:PEG:C2	1.93	0.82
1:F:42:MET:CE	1:F:72:HIS:CE1	2.62	0.82
1:A:279:THR:HG22	1:A:285:VAL:HG22	1.61	0.81
1:B:390:THR:O	1:B:394:THR:HG23	1.80	0.81
1:C:247:VAL:HG12	1:C:250:ILE:HD11	1.61	0.81
1:D:330:THR:O	1:D:334:THR:HG23	1.81	0.81
1:E:225:ILE:HD13	1:E:291:LEU:HD22	1.60	0.81
1:C:48:MET:HE1	1:C:50:THR:HG22	1.62	0.81
1:B:345:VAL:HG22	1:B:402:MET:HE1	1.63	0.81
1:E:90:ASN:HD21	1:E:93:LYS:CD	1.94	0.81
1:B:50:THR:HG21	3:B:639:HOH:O	1.82	0.79
1:F:393:GLN:O	1:F:397:THR:HG23	1.82	0.79
1:C:90:ASN:HD21	1:C:93:LYS:CE	1.94	0.79
1:E:393:GLN:O	1:E:397:THR:HG23	1.82	0.79
1:D:304:ILE:CG2	1:D:307:GLN:NE2	2.45	0.79
1:A:52:ARG:HD2	1:B:44:GLU:HB3	1.62	0.79
1:B:59:ASN:C	1:B:59:ASN:HD22	1.91	0.79
1:B:17:LEU:O	1:B:21:THR:CG2	2.31	0.78
1:F:308:ILE:HG22	1:F:333:ALA:HB1	1.64	0.78
1:D:52:ARG:HD3	3:E:445:HOH:O	1.82	0.78
1:A:44:GLU:HB3	1:B:52:ARG:HD2	1.66	0.78
1:E:212:VAL:CG1	1:E:217:ILE:O	2.32	0.77
1:E:321:VAL:HG12	1:E:344:LEU:HD23	1.65	0.77
1:B:323:GLU:OE1	1:B:329:THR:HG23	1.84	0.77
1:A:247:VAL:HB	1:A:265:ILE:HD11	1.65	0.77
1:F:247:VAL:HB	1:F:265:ILE:HD11	1.66	0.76
1:A:52:ARG:HD3	3:B:428:HOH:O	1.85	0.76
1:A:142:ILE:HD12	1:A:146:VAL:HG21	1.68	0.76
1:F:227:GLN:NE2	1:F:292:LEU:HD21	2.02	0.75
1:B:386:SER:O	1:B:390:THR:HG23	1.86	0.74
1:B:343:LEU:HD11	1:B:402:MET:HE2	1.68	0.74
1:A:62:VAL:HG21	1:B:424:VAL:HG12	1.67	0.74
1:F:219:LEU:CD1	1:F:243:ALA:HB1	2.15	0.74
1:B:42:MET:HE2	1:B:72:HIS:CE1	2.23	0.74
1:D:304:ILE:HG22	1:D:307:GLN:HE21	1.52	0.74
1:F:17:LEU:O	1:F:21:THR:HG23	1.88	0.74
1:F:224:ILE:HD11	1:F:300:VAL:HG23	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ARG:HG3	3:C:819:HOH:O	1.88	0.73
1:D:302:ALA:HB2	1:D:324:ARG:NH1	2.02	0.73
1:B:227:GLN:NE2	1:B:302:ALA:H	1.85	0.73
1:F:236:LEU:HD21	1:F:324:ARG:HD3	1.69	0.73
1:F:331:ILE:H	1:F:331:ILE:HD12	1.54	0.73
1:B:343:LEU:CD1	1:B:402:MET:HE2	2.19	0.73
1:D:160:ASN:HD21	2:D:425:PEG:H21	1.54	0.72
1:E:110:LEU:HD11	1:E:355:VAL:HG12	1.70	0.72
1:F:225:ILE:HD11	3:F:635:HOH:O	1.87	0.72
1:B:42:MET:HE3	1:B:42:MET:HA	1.71	0.72
1:A:393:GLN:O	1:A:397:THR:HG23	1.89	0.72
1:C:390:THR:O	1:C:394:THR:CG2	2.38	0.71
1:A:17:LEU:O	1:A:21:THR:HG23	1.90	0.71
1:E:146:VAL:HG13	1:E:182:PHE:CE1	2.25	0.71
1:F:204:VAL:HG21	1:F:324:ARG:HD2	1.72	0.71
1:C:278:VAL:HG12	1:C:279:THR:H	1.56	0.71
1:A:44:GLU:HG3	1:A:45:PRO:HD2	1.72	0.70
1:A:236:LEU:HD13	1:A:324:ARG:HD3	1.71	0.70
1:A:175:ARG:HD2	3:A:441:HOH:O	1.90	0.70
1:A:293:GLU:O	1:A:317:GLN:NE2	2.21	0.70
1:B:48:MET:HE1	1:B:68:TYR:HB3	1.72	0.70
1:B:42:MET:CE	1:B:72:HIS:CE1	2.75	0.69
1:B:90:ASN:ND2	1:B:93:LYS:H	1.90	0.69
1:B:146:VAL:HG13	1:B:182:PHE:CE1	2.27	0.69
1:B:227:GLN:HE21	1:B:302:ALA:H	1.38	0.69
1:B:330:THR:O	1:B:334:THR:CG2	2.40	0.69
1:F:116:LYS:NZ	1:F:156:ASP:OD2	2.25	0.69
1:D:144:GLN:HE21	1:E:150:LYS:NZ	1.91	0.69
1:D:304:ILE:HG22	1:D:307:GLN:NE2	2.06	0.69
1:E:212:VAL:HG12	1:E:217:ILE:O	1.90	0.69
1:E:14:ALA:CB	1:E:93:LYS:HE3	2.20	0.69
1:E:310:ALA:HB3	1:E:311:LYS:HE2	1.75	0.68
1:D:150:LYS:NZ	1:E:144:GLN:HE21	1.91	0.68
1:C:206:ILE:HD13	1:C:381:ARG:HA	1.76	0.68
1:C:337:LEU:O	1:C:342:VAL:HG13	1.93	0.68
1:D:205:THR:CG2	1:D:236:LEU:HD13	2.23	0.68
1:A:285:VAL:HG12	1:A:285:VAL:O	1.94	0.68
1:D:160:ASN:HD21	2:D:425:PEG:H22	1.59	0.68
1:A:236:LEU:HD13	1:A:324:ARG:CD	2.24	0.68
1:E:206:ILE:HD13	1:E:381:ARG:HA	1.76	0.68
1:E:298:ILE:HG23	1:E:320:ILE:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LYS:HZ3	1:B:144:GLN:HE21	1.42	0.67
1:E:90:ASN:HD21	1:E:93:LYS:CG	2.07	0.67
1:D:304:ILE:HG21	1:D:307:GLN:NE2	2.09	0.67
1:F:380:LEU:O	1:F:380:LEU:HD22	1.93	0.67
1:F:24:ILE:HG23	1:F:407:TYR:CD1	2.29	0.67
1:E:48:MET:HE1	1:E:50:THR:HG22	1.77	0.67
1:B:168:MET:HE3	1:B:169:ASP:N	2.09	0.67
1:A:132:GLU:OE2	3:A:517:HOH:O	2.13	0.66
1:C:240:MET:HE3	1:C:245:ALA:HB3	1.76	0.66
1:B:212:VAL:HG13	1:B:217:ILE:O	1.95	0.66
1:C:225:ILE:HD11	1:C:291:LEU:HG	1.76	0.66
1:A:236:LEU:HD13	1:A:324:ARG:NE	2.10	0.66
1:C:44:GLU:HB2	1:F:52:ARG:HD2	1.77	0.66
1:E:337:LEU:HB3	1:E:342:VAL:HG13	1.76	0.66
1:F:101:MET:CE	3:F:503:HOH:O	2.44	0.66
1:C:251:SER:HB2	1:C:291:LEU:HD23	1.78	0.65
1:E:90:ASN:ND2	1:E:93:LYS:CD	2.52	0.65
1:D:47:ARG:NH1	1:D:71:GLN:OE1	2.29	0.65
1:D:32:LEU:HD13	1:D:408:MET:CE	2.26	0.65
1:D:32:LEU:HD13	1:D:408:MET:HE3	1.79	0.65
1:A:17:LEU:O	1:A:21:THR:CG2	2.45	0.65
1:C:332:ASP:O	1:C:336:ILE:HD12	1.96	0.65
1:D:205:THR:HG22	1:D:236:LEU:HD13	1.79	0.65
1:A:204:VAL:HG11	1:A:324:ARG:HE	1.62	0.64
1:A:236:LEU:HB3	1:A:324:ARG:NH1	2.12	0.64
1:F:419:ARG:HH11	1:F:419:ARG:HG3	1.63	0.64
1:C:390:THR:O	1:C:394:THR:HG22	1.98	0.64
1:F:254:ASN:N	1:F:254:ASN:HD22	1.96	0.64
1:A:204:VAL:HB	1:A:236:LEU:HD11	1.79	0.64
1:B:330:THR:O	1:B:334:THR:HG23	1.96	0.64
1:E:319:SER:C	1:E:342:VAL:HG23	2.23	0.64
1:A:279:THR:HG22	1:A:285:VAL:CG2	2.27	0.64
1:C:321:VAL:HB	1:C:344:LEU:HD12	1.80	0.64
1:E:90:ASN:HD21	1:E:93:LYS:HG3	1.62	0.63
1:A:236:LEU:CB	1:A:324:ARG:NH1	2.61	0.63
1:E:227:GLN:C	1:E:302:ALA:HB2	2.23	0.63
1:F:32:LEU:HD13	1:F:408:MET:HE3	1.81	0.63
1:A:146:VAL:HG13	1:A:182:PHE:HE1	1.64	0.63
1:E:258:TYR:CE1	1:E:294:LYS:HB3	2.34	0.62
1:D:229:PHE:CE1	1:D:250:ILE:HD11	2.34	0.62
1:B:175:ARG:HD2	3:B:463:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ASN:HD21	2:C:425:PEG:C2	2.11	0.62
1:D:44:GLU:HB2	1:E:52:ARG:HD2	1.81	0.62
1:A:287:THR:OG1	1:A:290:GLU:HG3	1.99	0.62
1:B:393:GLN:O	1:B:397:THR:HG23	1.99	0.62
1:C:393:GLN:NE2	1:C:393:GLN:HA	2.15	0.62
1:A:279:THR:CG2	1:A:285:VAL:HG22	2.30	0.62
1:C:81:GLY:HA3	1:C:115:GLY:O	1.99	0.62
1:E:268:LEU:C	1:E:269:LEU:HD22	2.24	0.62
1:B:59:ASN:ND2	1:B:61:SER:H	1.98	0.61
1:F:405:ALA:O	1:F:409:THR:HG23	2.00	0.61
1:F:247:VAL:HG12	1:F:250:ILE:HD11	1.81	0.61
1:F:331:ILE:HD12	1:F:331:ILE:N	2.16	0.61
1:C:16:ASN:CA	1:C:19:LEU:HD23	2.30	0.61
3:A:438:HOH:O	1:B:52:ARG:HD3	2.01	0.61
1:F:32:LEU:HD13	1:F:408:MET:CE	2.31	0.61
1:E:219:LEU:HD21	1:E:240:MET:HE1	1.81	0.61
1:F:247:VAL:CG1	1:F:250:ILE:HD11	2.31	0.61
1:A:400:VAL:HG11	1:A:404:LEU:HD13	1.83	0.60
1:D:334:THR:HG22	1:D:403:ARG:HH21	1.66	0.60
1:F:313:ALA:HB3	1:F:336:ILE:HD13	1.83	0.60
1:A:46:GLN:OE1	1:A:73:ASN:HA	2.00	0.60
1:B:85:PHE:CE2	1:B:119:ILE:HD12	2.36	0.60
1:D:250:ILE:HG23	1:D:251:SER:N	2.15	0.60
1:A:204:VAL:HG21	1:A:324:ARG:HG2	1.84	0.60
1:D:224:ILE:HG21	1:D:240:MET:HG2	1.84	0.60
1:A:205:THR:HG22	1:A:236:LEU:HD23	1.80	0.60
1:B:90:ASN:C	1:B:90:ASN:HD22	2.08	0.60
1:B:146:VAL:HG13	1:B:182:PHE:HE1	1.65	0.60
1:A:24:ILE:HD11	1:A:331:ILE:HD11	1.84	0.59
1:E:321:VAL:CG1	1:E:344:LEU:HD23	2.31	0.59
1:A:52:ARG:CD	3:B:428:HOH:O	2.46	0.59
1:A:81:GLY:HA3	1:A:115:GLY:O	2.03	0.59
1:B:301:PRO:O	1:B:324:ARG:HD2	2.03	0.59
1:A:146:VAL:HG13	1:A:182:PHE:CE1	2.36	0.59
1:A:255:GLY:HA3	1:A:285:VAL:CG1	2.33	0.59
1:A:38:MET:HA	1:A:38:MET:CE	2.28	0.59
1:D:219:LEU:CD2	1:D:240:MET:CE	2.81	0.59
1:D:229:PHE:CZ	1:D:250:ILE:HD11	2.37	0.59
1:A:255:GLY:HA3	1:A:285:VAL:HG13	1.84	0.59
1:B:59:ASN:C	1:B:59:ASN:ND2	2.61	0.59
1:D:219:LEU:CD2	1:D:240:MET:HE3	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:THR:HG22	1:C:310:ALA:N	2.18	0.59
1:C:280:ASN:OD1	1:C:281:LEU:HD23	2.03	0.59
1:F:46:GLN:OE1	1:F:73:ASN:HA	2.03	0.59
1:A:224:ILE:HD13	1:A:240:MET:HG3	1.85	0.58
1:C:337:LEU:O	1:C:342:VAL:CG1	2.51	0.58
1:E:160:ASN:HD21	2:E:425:PEG:C2	2.15	0.58
1:E:393:GLN:O	1:E:397:THR:CG2	2.51	0.58
1:A:38:MET:HE1	1:A:41:LEU:HD12	1.84	0.58
1:B:59:ASN:HD22	1:B:60:GLY:N	2.01	0.58
1:C:393:GLN:HA	1:C:393:GLN:HE21	1.67	0.58
1:C:16:ASN:HA	1:C:19:LEU:HD23	1.84	0.58
1:C:247:VAL:CG1	1:C:250:ILE:HD11	2.34	0.58
1:C:309:THR:CG2	1:C:310:ALA:N	2.66	0.58
1:C:44:GLU:CB	1:F:52:ARG:HD2	2.33	0.58
1:D:337:LEU:HB3	1:D:342:VAL:HG22	1.86	0.58
1:D:219:LEU:HD21	1:D:240:MET:CE	2.34	0.58
1:E:201:ALA:O	1:E:205:THR:HG23	2.04	0.58
1:D:334:THR:CG2	1:D:403:ARG:HH21	2.17	0.58
1:F:352:ALA:O	1:F:355:VAL:HG12	2.03	0.58
1:D:194:GLN:NE2	3:D:441:HOH:O	2.37	0.58
1:E:47:ARG:HD2	1:E:71:GLN:OE1	2.04	0.58
1:A:59:ASN:C	1:A:59:ASN:HD22	2.10	0.57
1:C:303:ALA:C	1:C:304:ILE:HD13	2.30	0.57
1:E:224:ILE:HG21	1:E:240:MET:HG3	1.85	0.57
1:E:311:LYS:O	1:E:312:ASN:CG	2.47	0.57
1:F:219:LEU:HD13	1:F:243:ALA:CB	2.34	0.57
1:B:186:LYS:NZ	1:B:365:ASN:HD21	2.02	0.57
1:C:257:LEU:CD2	1:C:279:THR:HG22	2.35	0.57
1:D:205:THR:HG22	1:D:236:LEU:CD1	2.34	0.57
1:E:405:ALA:O	1:E:409:THR:HG23	2.05	0.57
1:A:236:LEU:HD22	1:A:324:ARG:HH21	1.68	0.57
1:A:386:SER:O	1:A:390:THR:HG23	2.04	0.57
1:F:101:MET:HE1	3:F:503:HOH:O	2.05	0.57
1:E:122:ASP:OD1	1:E:124:ARG:HD2	2.05	0.56
1:E:295:ASP:N	1:E:317:GLN:NE2	2.52	0.56
1:F:48:MET:HE1	1:F:68:TYR:HB3	1.87	0.56
1:E:295:ASP:CB	1:E:317:GLN:NE2	2.68	0.56
1:B:390:THR:O	1:B:394:THR:CG2	2.52	0.56
1:B:419:ARG:C	1:B:419:ARG:HD2	2.30	0.56
1:F:294:LYS:HB3	3:F:635:HOH:O	2.06	0.56
1:C:250:ILE:HD13	1:C:263:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:247:VAL:O	1:F:263:LEU:HD13	2.06	0.56
1:A:300:VAL:HG11	1:A:324:ARG:CD	2.36	0.56
1:E:404:LEU:HD22	1:E:404:LEU:O	2.05	0.56
1:B:47:ARG:HD2	1:B:71:GLN:OE1	2.05	0.56
1:C:249:GLY:HA3	1:C:291:LEU:HD11	1.86	0.56
1:C:390:THR:O	1:C:394:THR:HG23	2.06	0.56
1:A:263:LEU:O	1:A:265:ILE:HD12	2.05	0.55
1:D:349:LEU:HD22	1:D:391:ILE:HD12	1.86	0.55
1:C:309:THR:HG22	1:C:311:LYS:H	1.70	0.55
1:D:212:VAL:HG21	1:D:298:ILE:HD11	1.88	0.55
1:C:240:MET:HE3	1:C:245:ALA:CB	2.35	0.55
1:D:217:ILE:HG22	1:D:218:LYS:O	2.06	0.55
1:D:86:HIS:CE1	1:D:88:GLU:HG2	2.40	0.55
1:A:38:MET:HE3	1:A:424:VAL:HG21	1.89	0.55
1:F:247:VAL:HG21	1:F:265:ILE:HG13	1.89	0.55
1:A:424:VAL:HG12	1:B:62:VAL:HG11	1.88	0.55
1:C:333:ALA:O	1:C:337:LEU:HD13	2.07	0.55
1:A:300:VAL:HG11	1:A:324:ARG:CZ	2.36	0.55
1:E:16:ASN:O	1:E:20:SER:HB3	2.06	0.55
1:F:386:SER:O	1:F:390:THR:CG2	2.51	0.55
1:B:315:ASN:N	1:B:315:ASN:HD22	2.05	0.55
1:B:400:VAL:HG11	1:B:404:LEU:HD23	1.89	0.55
1:C:259:ASN:HB3	1:C:263:LEU:HD12	1.89	0.54
1:D:256:GLY:HA3	1:D:291:LEU:HD22	1.88	0.54
1:E:398:HIS:CG	1:E:408:MET:HE1	2.42	0.54
1:F:42:MET:HE2	1:F:72:HIS:CE1	2.42	0.54
1:F:101:MET:HE3	3:F:503:HOH:O	2.07	0.54
1:A:186:LYS:NZ	1:A:365:ASN:HD21	2.05	0.54
1:E:212:VAL:HG13	1:E:217:ILE:HB	1.89	0.54
1:B:329:THR:OG1	1:B:334:THR:HG22	2.06	0.54
1:C:48:MET:CE	1:C:50:THR:HG22	2.36	0.54
1:E:169:ASP:HB2	1:F:421:ARG:HD3	1.90	0.54
1:C:150:LYS:NZ	1:F:144:GLN:HE21	2.06	0.54
1:F:146:VAL:HG13	1:F:182:PHE:CE1	2.41	0.54
1:B:330:THR:O	1:B:334:THR:HG22	2.08	0.54
1:C:90:ASN:HD21	1:C:93:LYS:CD	2.19	0.54
1:E:389:GLU:OE2	1:E:393:GLN:OE1	2.26	0.54
3:C:437:HOH:O	1:F:52:ARG:HD3	2.08	0.53
1:D:160:ASN:ND2	2:D:425:PEG:H21	2.21	0.53
1:D:345:VAL:HG22	1:D:402:MET:HE1	1.89	0.53
1:E:160:ASN:HD21	2:E:425:PEG:H22	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:LEU:HD11	1:D:355:VAL:HG12	1.90	0.53
1:F:331:ILE:H	1:F:331:ILE:CD1	2.21	0.53
1:F:17:LEU:O	1:F:21:THR:CG2	2.55	0.53
1:E:186:LYS:NZ	1:E:365:ASN:HD21	2.07	0.53
1:D:405:ALA:O	1:D:409:THR:HG23	2.09	0.53
1:F:156:ASP:OD1	1:F:157:VAL:N	2.41	0.53
1:F:247:VAL:HG12	1:F:250:ILE:CD1	2.39	0.53
1:D:63:LYS:HE2	3:D:591:HOH:O	2.09	0.53
1:E:21:THR:O	1:E:25:ILE:HD13	2.08	0.53
1:E:337:LEU:HB3	1:E:342:VAL:CG1	2.39	0.53
1:B:214:LYS:HG2	1:B:392:TYR:CZ	2.44	0.53
1:A:236:LEU:HB3	1:A:324:ARG:CZ	2.38	0.53
1:B:386:SER:O	1:B:390:THR:CG2	2.57	0.53
1:C:84:ARG:NH1	1:C:156:ASP:OD1	2.42	0.53
1:E:48:MET:CE	1:E:50:THR:HG22	2.38	0.53
1:A:38:MET:CE	1:A:424:VAL:HG21	2.39	0.53
1:B:219:LEU:HD13	1:B:243:ALA:HB1	1.90	0.53
1:B:334:THR:HG21	1:B:403:ARG:HH21	1.73	0.53
1:D:186:LYS:NZ	1:D:365:ASN:HD21	2.06	0.52
1:A:240:MET:HA	1:A:240:MET:HE3	1.91	0.52
1:F:80:LYS:HG3	1:F:112:TYR:CD2	2.44	0.52
1:E:367:GLN:HE21	1:F:367:GLN:HE21	1.58	0.52
1:E:212:VAL:HG13	1:E:217:ILE:O	2.08	0.52
1:A:379:LYS:HE2	1:F:369:TYR:OH	2.10	0.52
1:C:390:THR:HG22	3:C:745:HOH:O	2.07	0.52
1:D:52:ARG:HD2	1:E:44:GLU:HB3	1.91	0.52
1:E:367:GLN:NE2	1:F:367:GLN:HE21	2.06	0.52
1:B:226:ILE:HD13	1:B:236:LEU:HB3	1.91	0.52
1:E:335:LYS:NZ	1:E:339:GLU:OE2	2.40	0.52
1:E:146:VAL:HG13	1:E:182:PHE:HE1	1.70	0.52
1:F:204:VAL:HG21	1:F:324:ARG:CD	2.40	0.52
1:A:150:LYS:NZ	1:B:144:GLN:NE2	2.51	0.52
1:A:273:ASP:HB2	1:A:277:MET:H	1.74	0.52
1:F:59:ASN:C	1:F:59:ASN:OD1	2.52	0.51
1:F:168:MET:HE3	1:F:169:ASP:HA	1.92	0.51
1:A:144:GLN:HE21	1:B:150:LYS:NZ	2.08	0.51
1:C:160:ASN:HD21	2:C:425:PEG:H21	1.74	0.51
1:D:17:LEU:HD12	1:D:93:LYS:HE3	1.91	0.51
1:A:219:LEU:CD2	1:A:240:MET:HE1	2.40	0.51
1:A:229:PHE:CD1	1:A:250:ILE:HD12	2.44	0.51
1:C:81:GLY:O	1:C:153:PRO:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:MET:SD	3:D:801:HOH:O	2.60	0.51
1:E:265:ILE:HA	1:E:268:LEU:HD12	1.92	0.51
1:B:186:LYS:HZ1	1:B:365:ASN:HD21	1.56	0.51
1:C:100:TRP:CZ3	1:C:348:ILE:HD12	2.45	0.51
1:A:393:GLN:HA	1:A:393:GLN:NE2	2.25	0.51
1:C:160:ASN:HD21	2:C:425:PEG:H22	1.76	0.51
1:D:205:THR:CG2	1:D:236:LEU:CD1	2.89	0.51
1:D:227:GLN:HB2	1:D:302:ALA:H	1.76	0.51
1:E:146:VAL:CG1	1:E:182:PHE:CE1	2.94	0.51
1:E:404:LEU:O	1:E:404:LEU:CD2	2.59	0.51
1:C:394:THR:HG21	3:C:482:HOH:O	2.09	0.51
1:E:330:THR:HG23	3:E:655:HOH:O	2.11	0.51
1:E:290:GLU:O	1:E:294:LYS:HG2	2.11	0.50
1:C:327:GLY:N	1:C:328:PRO:CD	2.75	0.50
1:F:42:MET:HE3	1:F:72:HIS:NE2	2.26	0.50
1:C:186:LYS:NZ	1:C:365:ASN:HD21	2.10	0.50
1:D:344:LEU:C	1:D:344:LEU:HD23	2.36	0.50
3:D:470:HOH:O	1:E:52:ARG:HD3	2.10	0.50
1:B:42:MET:HE2	1:B:72:HIS:HE1	1.73	0.50
1:C:302:ALA:O	1:C:303:ALA:HB3	2.11	0.50
1:F:81:GLY:HA3	1:F:115:GLY:O	2.12	0.50
1:A:204:VAL:HG11	1:A:324:ARG:NE	2.25	0.50
1:B:315:ASN:N	1:B:315:ASN:ND2	2.56	0.50
1:C:90:ASN:ND2	1:C:93:LYS:HD2	2.26	0.50
1:E:131:LEU:HD13	2:E:425:PEG:H42	1.92	0.50
1:A:24:ILE:HD11	1:A:331:ILE:CD1	2.42	0.49
1:E:404:LEU:HD22	1:E:408:MET:HG3	1.94	0.49
1:C:306:ASN:N	1:C:306:ASN:OD1	2.45	0.49
1:A:236:LEU:CB	1:A:324:ARG:CZ	2.90	0.49
1:C:186:LYS:HZ1	1:C:365:ASN:HD21	1.60	0.49
1:C:405:ALA:O	1:C:409:THR:HG23	2.12	0.49
1:D:345:VAL:HA	1:D:402:MET:CE	2.43	0.49
1:E:48:MET:HE3	1:E:48:MET:C	2.37	0.49
1:F:224:ILE:HD12	1:F:226:ILE:HG13	1.94	0.49
1:F:308:ILE:HG22	1:F:333:ALA:CB	2.40	0.49
1:C:90:ASN:ND2	1:C:93:LYS:CD	2.76	0.49
1:D:150:LYS:HZ2	1:E:144:GLN:HE21	1.59	0.49
1:A:59:ASN:C	1:A:59:ASN:ND2	2.69	0.49
1:D:219:LEU:HD23	1:D:240:MET:HE3	1.93	0.49
1:C:386:SER:O	1:C:390:THR:HG23	2.11	0.49
1:D:304:ILE:HD13	1:D:304:ILE:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ARG:NH1	1:B:156:ASP:OD1	2.46	0.49
1:A:386:SER:O	1:A:390:THR:CG2	2.61	0.49
1:B:316:ILE:O	1:B:340:ARG:NH1	2.44	0.49
1:B:375:GLU:HB3	3:B:482:HOH:O	2.13	0.49
1:C:257:LEU:HB2	1:C:263:LEU:HD21	1.95	0.49
1:C:40:GLU:OE1	1:C:43:LYS:NZ	2.26	0.48
1:C:340:ARG:HD3	3:C:625:HOH:O	2.13	0.48
1:C:201:ALA:HB2	1:C:324:ARG:HH22	1.76	0.48
1:C:304:ILE:HG22	1:C:305:SER:H	1.78	0.48
1:E:330:THR:CG2	3:E:655:HOH:O	2.61	0.48
1:D:220:GLN:O	1:D:244:GLY:O	2.32	0.48
1:D:393:GLN:O	1:D:397:THR:HG23	2.13	0.48
1:F:42:MET:HE3	1:F:72:HIS:CE1	2.47	0.48
1:B:90:ASN:HD21	1:B:93:LYS:H	1.61	0.48
1:F:247:VAL:CB	1:F:265:ILE:HD11	2.40	0.48
1:B:308:ILE:HB	1:B:329:THR:HB	1.96	0.48
1:C:19:LEU:HD22	1:C:19:LEU:H	1.77	0.48
1:D:304:ILE:HD13	1:D:304:ILE:H	1.77	0.48
1:D:232:ALA:O	1:D:236:LEU:HD23	2.14	0.48
1:A:14:ALA:HB1	1:A:90:ASN:HD21	1.79	0.48
1:A:38:MET:CE	1:A:41:LEU:HD12	2.43	0.48
1:A:302:ALA:HB2	1:A:324:ARG:HD2	1.95	0.48
1:D:227:GLN:HE21	1:D:288:ASN:HD22	1.60	0.48
1:D:404:LEU:O	1:D:404:LEU:HD22	2.14	0.48
1:A:257:LEU:HG	1:A:279:THR:HG23	1.94	0.47
1:D:44:GLU:CB	1:E:52:ARG:HD2	2.44	0.47
1:E:313:ALA:HB1	1:E:336:ILE:HG21	1.95	0.47
1:B:252:ASP:OD2	1:B:278:VAL:O	2.32	0.47
1:C:175:ARG:NH2	1:E:176:GLU:OE2	2.36	0.47
1:B:168:MET:HE3	1:B:169:ASP:CA	2.44	0.47
1:D:302:ALA:HB2	1:D:324:ARG:HH12	1.75	0.47
1:A:393:GLN:HA	1:A:393:GLN:HE21	1.78	0.47
1:E:265:ILE:N	1:E:266:PRO:CD	2.78	0.47
1:F:24:ILE:HD13	1:F:407:TYR:CE1	2.49	0.47
1:F:219:LEU:CD1	1:F:243:ALA:CB	2.88	0.47
1:B:279:THR:O	1:B:285:VAL:HG21	2.14	0.47
1:D:85:PHE:CE2	1:D:119:ILE:HD12	2.49	0.47
1:E:232:ALA:HB1	1:E:324:ARG:HD3	1.97	0.47
1:F:42:MET:HE2	1:F:72:HIS:HE1	1.79	0.47
1:A:219:LEU:HD21	1:A:240:MET:HE1	1.97	0.47
1:C:169:ASP:OD1	1:D:421:ARG:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:ASP:O	1:C:285:VAL:HG23	2.15	0.47
1:D:257:LEU:N	1:D:257:LEU:HD22	2.29	0.47
1:E:302:ALA:O	1:E:304:ILE:N	2.47	0.47
1:A:205:THR:HG21	1:A:239:PHE:CG	2.49	0.47
1:B:220:GLN:HG2	3:B:811:HOH:O	2.14	0.47
1:E:194:GLN:NE2	3:E:838:HOH:O	2.48	0.47
1:B:50:THR:HB	1:B:68:TYR:CD1	2.49	0.47
1:E:81:GLY:O	1:E:153:PRO:HA	2.14	0.47
1:D:32:LEU:HD13	1:D:408:MET:HE2	1.97	0.46
1:E:175:ARG:HD2	3:E:448:HOH:O	2.15	0.46
1:D:219:LEU:HD23	1:D:240:MET:CE	2.45	0.46
1:E:73:ASN:O	1:E:113:GLY:HA3	2.15	0.46
1:F:405:ALA:O	1:F:409:THR:CG2	2.63	0.46
1:A:421:ARG:HD2	1:F:169:ASP:OD1	2.15	0.46
1:D:248:ILE:CG2	1:D:258:TYR:CE1	2.98	0.46
1:E:186:LYS:HZ1	1:E:365:ASN:HD21	1.62	0.46
1:E:226:ILE:HA	1:E:300:VAL:HG13	1.96	0.46
1:E:296:CYS:SG	1:E:318:ALA:HB2	2.56	0.46
1:F:335:LYS:O	1:F:339:GLU:HG2	2.15	0.46
1:C:201:ALA:HB1	1:C:235:PHE:CD1	2.50	0.46
1:C:86:HIS:CG	1:C:87:PRO:HD2	2.51	0.46
1:E:81:GLY:HA3	1:E:115:GLY:O	2.15	0.46
1:F:24:ILE:CG2	1:F:407:TYR:CD1	2.97	0.46
1:C:278:VAL:HG12	1:C:279:THR:N	2.28	0.46
1:F:249:GLY:C	1:F:250:ILE:HD12	2.41	0.46
1:C:90:ASN:ND2	1:C:93:LYS:CE	2.72	0.46
1:C:225:ILE:HD12	1:C:291:LEU:CD1	2.45	0.46
1:D:229:PHE:CD1	1:D:250:ILE:HD11	2.51	0.46
1:A:185:GLY:HA2	1:A:196:ARG:HD3	1.98	0.46
1:A:186:LYS:HZ1	1:A:365:ASN:HD21	1.63	0.46
1:C:227:GLN:HA	1:C:251:SER:HB3	1.98	0.46
1:D:32:LEU:CD1	1:D:408:MET:HE2	2.46	0.46
1:D:48:MET:HE1	1:D:68:TYR:HB3	1.97	0.46
1:F:232:ALA:O	1:F:236:LEU:HD22	2.16	0.46
1:F:264:ASP:O	1:F:268:LEU:HD13	2.15	0.46
1:B:168:MET:HE3	1:B:169:ASP:HA	1.98	0.46
1:C:224:ILE:HD13	1:C:240:MET:HG3	1.98	0.46
1:D:345:VAL:HA	1:D:402:MET:HE3	1.98	0.46
1:B:80:LYS:HD2	1:B:152:ILE:HB	1.98	0.46
1:E:90:ASN:HD22	1:E:93:LYS:HD2	1.74	0.46
1:E:292:LEU:HD13	1:E:307:GLN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:LEU:O	1:E:342:VAL:HG12	2.16	0.46
1:F:47:ARG:HD2	1:F:71:GLN:OE1	2.16	0.46
1:F:224:ILE:HD11	1:F:300:VAL:CG2	2.41	0.46
1:A:236:LEU:HD22	1:A:324:ARG:CZ	2.44	0.45
1:D:325:ALA:O	1:D:328:PRO:HD3	2.16	0.45
1:B:215:LYS:NZ	1:B:341:GLY:O	2.49	0.45
1:D:408:MET:O	1:D:412:ARG:HB2	2.16	0.45
1:E:219:LEU:CD2	1:E:240:MET:HE1	2.45	0.45
1:E:311:LYS:O	1:E:312:ASN:CB	2.64	0.45
1:C:100:TRP:HZ3	1:C:348:ILE:HD12	1.80	0.45
1:D:256:GLY:C	1:D:257:LEU:HD22	2.42	0.45
1:D:279:THR:HG23	1:D:285:VAL:CG2	2.46	0.45
1:F:101:MET:O	1:F:102:THR:C	2.60	0.45
1:A:196:ARG:HG2	1:A:197:GLU:N	2.30	0.45
1:D:144:GLN:HE21	1:E:150:LYS:HZ3	1.61	0.45
1:F:196:ARG:HD2	3:F:634:HOH:O	2.16	0.45
1:D:280:ASN:CG	1:D:281:LEU:HD22	2.42	0.45
1:F:219:LEU:O	1:F:245:ALA:HB2	2.16	0.45
1:F:372:SER:OG	1:F:375:GLU:HG3	2.17	0.45
1:C:250:ILE:O	1:C:250:ILE:HG22	2.17	0.45
1:D:214:LYS:HD2	1:D:392:TYR:CE2	2.52	0.45
1:F:307:GLN:OE1	1:F:307:GLN:CA	2.64	0.45
1:A:59:ASN:ND2	1:A:61:SER:H	2.15	0.45
1:E:327:GLY:N	1:E:328:PRO:CD	2.79	0.45
1:F:217:ILE:HD11	1:F:222:ALA:HB2	1.99	0.45
1:A:7:SER:HB3	1:A:10:GLU:OE1	2.17	0.45
1:A:212:VAL:HG13	1:A:217:ILE:O	2.17	0.45
1:A:214:LYS:NZ	1:A:389:GLU:OE1	2.41	0.45
1:D:205:THR:HG23	1:D:236:LEU:HD13	1.97	0.45
1:A:22:GLN:O	1:A:25:ILE:HG22	2.17	0.45
1:C:255:GLY:O	1:C:279:THR:HG21	2.17	0.45
1:E:63:LYS:NZ	3:E:779:HOH:O	2.49	0.45
1:E:160:ASN:HD21	2:E:425:PEG:H21	1.81	0.45
3:A:428:HOH:O	1:B:50:THR:HG23	2.16	0.44
1:B:352:ALA:O	1:B:355:VAL:HG22	2.18	0.44
1:C:268:LEU:O	1:C:272:ARG:HG3	2.16	0.44
1:D:73:ASN:O	1:D:113:GLY:HA3	2.17	0.44
1:B:86:HIS:HB3	1:B:89:VAL:HG23	1.98	0.44
1:E:408:MET:O	1:E:411:ILE:HD12	2.17	0.44
1:B:218:LYS:NZ	3:B:586:HOH:O	2.43	0.44
1:C:82:GLY:O	1:C:116:LYS:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:ALA:O	1:D:337:LEU:HD12	2.18	0.44
1:B:19:LEU:O	1:B:23:THR:HG23	2.17	0.44
1:C:247:VAL:HB	1:C:265:ILE:HD11	1.99	0.44
1:C:333:ALA:O	1:C:337:LEU:CD1	2.66	0.44
1:D:62:VAL:HG11	1:E:424:VAL:HG12	1.97	0.44
1:D:150:LYS:HZ3	1:E:144:GLN:HE21	1.66	0.44
1:E:305:SER:O	1:E:307:GLN:HG3	2.18	0.44
1:E:312:ASN:C	1:E:316:ILE:HD12	2.41	0.44
1:F:241:HIS:CE1	1:F:266:PRO:HD3	2.53	0.44
1:E:303:ALA:HA	1:E:325:ALA:HB2	1.99	0.44
1:F:85:PHE:CE2	1:F:119:ILE:HD12	2.53	0.44
1:A:85:PHE:HB3	1:A:123:PRO:HG3	1.99	0.44
1:C:248:ILE:HG22	1:C:249:GLY:N	2.32	0.44
1:E:250:ILE:HG22	1:E:251:SER:N	2.32	0.44
1:E:405:ALA:O	1:E:409:THR:CG2	2.65	0.44
1:C:144:GLN:HE21	1:F:150:LYS:NZ	2.16	0.44
1:F:80:LYS:CG	1:F:112:TYR:CD2	3.01	0.44
1:F:186:LYS:NZ	1:F:365:ASN:HD21	2.15	0.44
1:C:257:LEU:N	1:C:257:LEU:HD23	2.33	0.43
1:C:201:ALA:O	1:C:205:THR:HG23	2.18	0.43
1:E:240:MET:HE3	1:E:240:MET:HA	2.00	0.43
1:F:224:ILE:HG22	1:F:247:VAL:HA	1.99	0.43
1:A:7:SER:HB3	1:A:10:GLU:CD	2.43	0.43
1:A:229:PHE:CE1	1:A:250:ILE:HD12	2.53	0.43
1:A:236:LEU:HB2	1:A:324:ARG:NH1	2.33	0.43
1:B:312:ASN:HD22	1:B:312:ASN:H	1.66	0.43
1:D:286:ILE:HD12	1:D:290:GLU:HG3	2.01	0.43
1:A:273:ASP:OD2	1:A:277:MET:HB2	2.18	0.43
1:D:212:VAL:CG2	1:D:298:ILE:HD11	2.48	0.43
1:E:198:THR:HG22	1:E:198:THR:O	2.19	0.43
1:E:215:LYS:HB3	1:E:217:ILE:HD12	1.99	0.43
1:F:308:ILE:O	1:F:330:THR:HG23	2.19	0.43
1:A:63:LYS:HG3	1:A:65:PHE:CE1	2.53	0.43
1:E:344:LEU:C	1:E:344:LEU:HD22	2.43	0.43
1:E:110:LEU:HD11	1:E:355:VAL:CG1	2.45	0.43
1:B:400:VAL:CG1	1:B:404:LEU:HD23	2.48	0.43
1:C:175:ARG:HD2	3:C:444:HOH:O	2.18	0.43
1:C:250:ILE:CD1	1:C:263:LEU:HD22	2.47	0.43
1:D:324:ARG:O	1:D:324:ARG:HG2	2.19	0.43
1:C:173:ARG:CG	3:C:819:HOH:O	2.58	0.43
1:D:325:ALA:CB	1:D:326:ASN:HB2	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ARG:CG	1:B:156:ASP:OD1	2.67	0.43
1:B:168:MET:HE3	1:B:168:MET:C	2.44	0.43
1:E:84:ARG:HG3	1:E:156:ASP:CG	2.44	0.43
1:C:90:ASN:ND2	1:C:93:LYS:HE3	2.14	0.43
1:C:259:ASN:O	1:C:260:PRO:C	2.62	0.43
1:F:259:ASN:HB3	1:F:263:LEU:HD12	2.01	0.43
1:C:16:ASN:N	1:C:19:LEU:HD22	2.29	0.42
1:C:215:LYS:C	1:C:217:ILE:H	2.27	0.42
1:C:408:MET:O	1:C:412:ARG:HB2	2.19	0.42
1:F:224:ILE:HD13	1:F:225:ILE:N	2.34	0.42
1:F:349:LEU:HD11	1:F:384:MET:HE1	2.01	0.42
1:B:90:ASN:HD21	1:B:93:LYS:HG3	1.84	0.42
1:B:412:ARG:CG	1:B:416:GLU:OE2	2.67	0.42
1:E:289:GLU:OE2	1:E:289:GLU:N	2.50	0.42
1:A:90:ASN:ND2	1:A:93:LYS:HB3	2.34	0.42
1:B:227:GLN:HE21	1:B:302:ALA:N	2.12	0.42
1:B:375:GLU:OE2	3:B:482:HOH:O	2.21	0.42
1:C:264:ASP:O	1:C:268:LEU:HD12	2.19	0.42
1:E:268:LEU:O	1:E:269:LEU:HD13	2.19	0.42
1:F:198:THR:OG1	1:F:202:GLN:NE2	2.51	0.42
1:A:150:LYS:HD3	1:B:144:GLN:HE22	1.85	0.42
3:A:428:HOH:O	1:B:50:THR:CG2	2.67	0.42
1:C:257:LEU:HD21	1:C:279:THR:HG22	2.02	0.42
1:C:265:ILE:HG22	1:C:269:LEU:HD22	2.00	0.42
1:D:59:ASN:OD1	1:D:59:ASN:C	2.63	0.42
1:E:268:LEU:O	1:E:269:LEU:HD22	2.19	0.42
1:A:374:GLU:CD	1:A:374:GLU:H	2.27	0.42
1:B:325:ALA:HA	1:B:347:ASP:OD1	2.19	0.42
1:C:252:ASP:O	1:C:253:ALA:C	2.63	0.42
1:D:47:ARG:NH2	1:D:74:ASP:OD2	2.52	0.42
1:D:316:ILE:O	1:D:340:ARG:NH2	2.52	0.42
1:E:173:ARG:HH11	1:E:173:ARG:HA	1.85	0.42
1:E:206:ILE:HG21	1:E:384:MET:HB2	2.01	0.42
1:B:344:LEU:O	1:B:402:MET:HE3	2.20	0.42
1:E:101:MET:HE1	1:E:355:VAL:HG22	2.02	0.42
1:F:199:ALA:HB2	1:F:357:VAL:HG21	2.01	0.42
1:B:246:LYS:NZ	3:B:437:HOH:O	2.52	0.42
1:D:79:THR:HA	1:D:113:GLY:O	2.20	0.42
1:A:59:ASN:HD22	1:A:60:GLY:N	2.17	0.42
1:A:150:LYS:HZ2	1:B:144:GLN:HE21	1.60	0.42
1:C:44:GLU:HB2	1:F:52:ARG:CD	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:HIS:ND1	1:D:88:GLU:HG2	2.35	0.42
1:F:327:GLY:N	1:F:328:PRO:CD	2.83	0.42
1:C:19:LEU:HD22	1:C:19:LEU:N	2.34	0.41
1:C:48:MET:HE3	1:C:48:MET:C	2.45	0.41
1:F:217:ILE:HD11	1:F:222:ALA:CB	2.50	0.41
1:A:21:THR:HG21	1:A:100:TRP:HE1	1.85	0.41
1:B:81:GLY:HA3	1:B:115:GLY:O	2.20	0.41
1:B:343:LEU:HD12	1:B:402:MET:HE2	2.00	0.41
1:E:112:TYR:HH	1:E:362:TRP:CG	2.38	0.41
1:F:80:LYS:HG3	1:F:112:TYR:CE2	2.55	0.41
1:F:307:GLN:OE1	1:F:307:GLN:HA	2.20	0.41
1:C:268:LEU:HD23	1:C:278:VAL:CG1	2.41	0.41
1:D:324:ARG:O	1:D:325:ALA:HB2	2.21	0.41
1:E:299:LEU:HD22	1:E:300:VAL:N	2.35	0.41
1:E:372:SER:O	1:E:376:VAL:HG23	2.20	0.41
1:F:409:THR:HB	3:F:843:HOH:O	2.20	0.41
1:B:336:ILE:O	1:B:340:ARG:HG3	2.20	0.41
1:C:309:THR:CG2	1:C:310:ALA:H	2.32	0.41
1:C:273:ASP:HB3	1:C:277:MET:H	1.85	0.41
1:C:323:GLU:OE2	1:C:344:LEU:HD21	2.19	0.41
1:E:28:ALA:HB1	1:E:411:ILE:HD11	2.03	0.41
1:E:298:ILE:HA	1:E:320:ILE:O	2.21	0.41
1:B:421:ARG:HD2	1:D:169:ASP:OD1	2.21	0.41
1:C:214:LYS:HD3	1:C:392:TYR:CZ	2.56	0.41
1:E:90:ASN:ND2	1:E:93:LYS:CG	2.79	0.41
1:A:423:TRP:CD1	1:A:423:TRP:N	2.87	0.41
1:D:300:VAL:HG12	1:D:324:ARG:HH21	1.86	0.41
1:F:79:THR:O	1:F:151:ASP:HA	2.21	0.41
1:A:171:TYR:OH	1:A:175:ARG:NH1	2.54	0.41
1:B:390:THR:HG21	3:B:729:HOH:O	2.21	0.41
1:F:257:LEU:N	1:F:257:LEU:HD23	2.36	0.41
1:F:288:ASN:HD22	1:F:288:ASN:N	2.19	0.41
1:B:308:ILE:HG22	1:B:333:ALA:HB1	2.02	0.41
1:D:49:LEU:HD13	1:D:142:ILE:HG22	2.03	0.41
1:D:88:GLU:O	1:D:89:VAL:C	2.64	0.41
1:F:80:LYS:CG	1:F:112:TYR:CE2	3.04	0.41
1:C:50:THR:HG23	3:F:430:HOH:O	2.21	0.40
1:E:84:ARG:O	1:E:118:GLY:HA2	2.21	0.40
1:C:303:ALA:HB1	1:C:304:ILE:HG12	2.03	0.40
1:F:257:LEU:O	1:F:263:LEU:HD21	2.22	0.40
1:A:84:ARG:O	1:A:118:GLY:HA2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ARG:HD2	3:A:536:HOH:O	2.20	0.40
1:D:26:LYS:O	1:D:30:ARG:HB2	2.21	0.40
1:C:230:GLY:O	1:C:234:SER:OG	2.34	0.40
1:C:259:ASN:HB3	1:C:263:LEU:CD1	2.50	0.40
1:D:226:ILE:HG23	1:D:324:ARG:NH2	2.37	0.40
1:A:253:ALA:H	1:A:277:MET:HE1	1.86	0.40
1:B:17:LEU:HD22	1:B:21:THR:CG2	2.51	0.40
1:B:84:ARG:O	1:B:118:GLY:HA2	2.22	0.40
1:B:173:ARG:NH2	3:B:549:HOH:O	2.53	0.40
1:D:380:LEU:HD22	1:D:384:MET:HG2	2.03	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	416/424 (98%)	400 (96%)	13 (3%)	3 (1%)	18	23
1	B	407/424 (96%)	396 (97%)	10 (2%)	1 (0%)	43	55
1	C	407/424 (96%)	376 (92%)	19 (5%)	12 (3%)	3	2
1	D	402/424 (95%)	383 (95%)	17 (4%)	2 (0%)	24	31
1	E	392/424 (92%)	360 (92%)	27 (7%)	5 (1%)	9	10
1	F	391/424 (92%)	367 (94%)	22 (6%)	2 (0%)	24	31
All	All	2415/2544 (95%)	2282 (94%)	108 (4%)	25 (1%)	12	15

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	ASP
1	C	248	ILE

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Mol	Chain	Res	Type
1	C	283	THR
1	E	303	ALA
1	E	306	ASN
1	F	303	ALA
1	A	312	ASN
1	B	278	VAL
1	C	302	ALA
1	C	311	LYS
1	C	312	ASN
1	D	303	ALA
1	D	304	ILE
1	E	312	ASN
1	C	280	ASN
1	C	303	ALA
1	E	232	ALA
1	F	268	LEU
1	C	216	GLY
1	C	279	THR
1	C	285	VAL
1	E	259	ASN
1	A	278	VAL
1	C	278	VAL
1	C	259	ASN

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	346/351 (99%)	309 (89%)	37 (11%)	6	8
1	B	338/351 (96%)	301 (89%)	37 (11%)	6	7
1	C	338/351 (96%)	301 (89%)	37 (11%)	6	7
1	D	333/351 (95%)	306 (92%)	27 (8%)	11	14
1	E	324/351 (92%)	283 (87%)	41 (13%)	4	5
1	F	324/351 (92%)	286 (88%)	38 (12%)	5	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2003/2106 (95%)	1786 (89%)	217 (11%)	6 7

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	13	GLU
1	A	21	THR
1	A	26	LYS
1	A	32	LEU
1	A	38	MET
1	A	41	LEU
1	A	49	LEU
1	A	50	THR
1	A	59	ASN
1	A	62	VAL
1	A	63	LYS
1	A	84	ARG
1	A	92	GLU
1	A	93	LYS
1	A	146	VAL
1	A	168	MET
1	A	173	ARG
1	A	188	LEU
1	A	205	THR
1	A	212	VAL
1	A	219	LEU
1	A	236	LEU
1	A	265	ILE
1	A	272	ARG
1	A	279	THR
1	A	293	GLU
1	A	299	LEU
1	A	316	ILE
1	A	344	LEU
1	A	382	SER
1	A	390	THR
1	A	397	THR
1	A	404	LEU
1	A	411	ILE
1	A	419	ARG
1	A	424	VAL

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Mol	Chain	Res	Type
1	B	17	LEU
1	B	21	THR
1	B	24	ILE
1	B	32	LEU
1	B	41	LEU
1	B	49	LEU
1	B	50	THR
1	B	56	LYS
1	B	59	ASN
1	B	88	GLU
1	B	90	ASN
1	B	146	VAL
1	B	168	MET
1	B	173	ARG
1	B	188	LEU
1	B	212	VAL
1	B	219	LEU
1	B	220	GLN
1	B	236	LEU
1	B	269	LEU
1	B	270	ASP
1	B	278	VAL
1	B	279	THR
1	B	299	LEU
1	B	312	ASN
1	B	316	ILE
1	B	329	THR
1	B	331	ILE
1	B	334	THR
1	B	344	LEU
1	B	357	VAL
1	B	390	THR
1	B	394	THR
1	B	397	THR
1	B	399	LYS
1	B	411	ILE
1	B	419	ARG
1	C	17	LEU
1	C	19	LEU
1	C	32	LEU
1	C	41	LEU
1	C	48	MET

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Mol	Chain	Res	Type
1	C	49	LEU
1	C	50	THR
1	C	52	ARG
1	C	56	LYS
1	C	83	VAL
1	C	175	ARG
1	C	188	LEU
1	C	209	GLU
1	C	214	LYS
1	C	219	LEU
1	C	220	GLN
1	C	225	ILE
1	C	234	SER
1	C	236	LEU
1	C	250	ILE
1	C	271	LYS
1	C	281	LEU
1	C	282	PHE
1	C	286	ILE
1	C	299	LEU
1	C	304	ILE
1	C	305	SER
1	C	306	ASN
1	C	336	ILE
1	C	342	VAL
1	C	367	GLN
1	C	380	LEU
1	C	389	GLU
1	C	390	THR
1	C	394	THR
1	C	404	LEU
1	C	409	THR
1	D	17	LEU
1	D	30	ARG
1	D	32	LEU
1	D	41	LEU
1	D	49	LEU
1	D	56	LYS
1	D	88	GLU
1	D	93	LYS
1	D	146	VAL
1	D	188	LEU

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Mol	Chain	Res	Type
1	D	218	LYS
1	D	219	LEU
1	D	248	ILE
1	D	250	ILE
1	D	251	SER
1	D	271	LYS
1	D	279	THR
1	D	299	LEU
1	D	304	ILE
1	D	317	GLN
1	D	326	ASN
1	D	342	VAL
1	D	358	SER
1	D	380	LEU
1	D	404	LEU
1	D	409	THR
1	D	411	ILE
1	E	12	LYS
1	E	13	GLU
1	E	15	LEU
1	E	30	ARG
1	E	32	LEU
1	E	41	LEU
1	E	48	MET
1	E	49	LEU
1	E	50	THR
1	E	84	ARG
1	E	89	VAL
1	E	95	LYS
1	E	100	TRP
1	E	146	VAL
1	E	173	ARG
1	E	175	ARG
1	E	188	LEU
1	E	219	LEU
1	E	231	ASN
1	E	236	LEU
1	E	251	SER
1	E	254	ASN
1	E	267	TYR
1	E	291	LEU
1	E	294	LYS

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Mol	Chain	Res	Type
1	E	299	LEU
1	E	304	ILE
1	E	311	LYS
1	E	317	GLN
1	E	326	ASN
1	E	344	LEU
1	E	374	GLU
1	E	380	LEU
1	E	393	GLN
1	E	397	THR
1	E	404	LEU
1	E	409	THR
1	E	411	ILE
1	E	412	ARG
1	E	419	ARG
1	E	424	VAL
1	F	16	ASN
1	F	21	THR
1	F	31	LYS
1	F	32	LEU
1	F	41	LEU
1	F	49	LEU
1	F	56	LYS
1	F	80	LYS
1	F	146	VAL
1	F	168	MET
1	F	188	LEU
1	F	194	GLN
1	F	197	GLU
1	F	217	ILE
1	F	219	LEU
1	F	220	GLN
1	F	223	ARG
1	F	224	ILE
1	F	236	LEU
1	F	247	VAL
1	F	248	ILE
1	F	254	ASN
1	F	257	LEU
1	F	294	LYS
1	F	299	LEU
1	F	307	GLN

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Mol	Chain	Res	Type
1	F	316	ILE
1	F	326	ASN
1	F	331	ILE
1	F	378	GLU
1	F	380	LEU
1	F	381	ARG
1	F	384	MET
1	F	390	THR
1	F	397	THR
1	F	404	LEU
1	F	409	THR
1	F	411	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	59	ASN
1	A	90	ASN
1	A	144	GLN
1	A	194	GLN
1	A	227	GLN
1	A	231	ASN
1	A	306	ASN
1	A	312	ASN
1	A	338	ASN
1	A	365	ASN
1	A	367	GLN
1	A	393	GLN
1	B	59	ASN
1	B	90	ASN
1	B	144	GLN
1	B	194	GLN
1	B	202	GLN
1	B	220	GLN
1	B	227	GLN
1	B	231	ASN
1	B	254	ASN
1	B	288	ASN
1	B	312	ASN
1	B	315	ASN
1	B	317	GLN

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Mol	Chain	Res	Type
1	B	326	ASN
1	B	365	ASN
1	B	367	GLN
1	B	393	GLN
1	C	90	ASN
1	C	144	GLN
1	C	194	GLN
1	C	202	GLN
1	C	221	ASN
1	C	227	GLN
1	C	254	ASN
1	C	280	ASN
1	C	288	ASN
1	C	307	GLN
1	C	312	ASN
1	C	317	GLN
1	C	326	ASN
1	C	365	ASN
1	C	367	GLN
1	C	393	GLN
1	D	144	GLN
1	D	160	ASN
1	D	194	GLN
1	D	202	GLN
1	D	220	GLN
1	D	221	ASN
1	D	227	GLN
1	D	231	ASN
1	D	288	ASN
1	D	307	GLN
1	D	312	ASN
1	D	365	ASN
1	E	90	ASN
1	E	144	GLN
1	E	162	GLN
1	E	194	GLN
1	E	202	GLN
1	E	254	ASN
1	E	259	ASN
1	E	307	GLN
1	E	312	ASN
1	E	317	GLN

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Mol	Chain	Res	Type
1	E	365	ASN
1	E	367	GLN
1	F	144	GLN
1	F	202	GLN
1	F	221	ASN
1	F	227	GLN
1	F	241	HIS
1	F	254	ASN
1	F	259	ASN
1	F	288	ASN
1	F	312	ASN
1	F	326	ASN
1	F	365	ASN
1	F	393	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	F	425	-	6,6,6	0.42	0	5,5,5	0.31	0
2	PEG	A	425	-	6,6,6	0.52	0	5,5,5	0.72	0
2	PEG	D	425	-	6,6,6	0.53	0	5,5,5	0.53	0
2	PEG	C	425	-	6,6,6	0.39	0	5,5,5	0.77	0
2	PEG	E	425	-	6,6,6	0.68	0	5,5,5	0.48	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	F	425	-	-	1/4/4/4	-
2	PEG	A	425	-	-	2/4/4/4	-
2	PEG	D	425	-	-	3/4/4/4	-
2	PEG	C	425	-	-	2/4/4/4	-
2	PEG	E	425	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	425	PEG	O2-C3-C4-O4
2	F	425	PEG	O2-C3-C4-O4
2	C	425	PEG	O1-C1-C2-O2
2	A	425	PEG	O1-C1-C2-O2
2	E	425	PEG	O2-C3-C4-O4
2	D	425	PEG	C1-C2-O2-C3
2	E	425	PEG	C4-C3-O2-C2
2	A	425	PEG	C1-C2-O2-C3
2	C	425	PEG	O2-C3-C4-O4
2	D	425	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	425	PEG	4	0
2	C	425	PEG	3	0
2	E	425	PEG	4	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	418/424 (98%)	-0.27	4 (0%) 79 80	26, 40, 64, 80	0
1	B	409/424 (96%)	-0.23	2 (0%) 87 87	27, 44, 69, 82	0
1	C	409/424 (96%)	0.27	34 (8%) 17 19	30, 48, 104, 114	0
1	D	406/424 (95%)	0.11	8 (1%) 65 66	29, 51, 83, 99	0
1	E	396/424 (93%)	0.38	38 (9%) 13 15	30, 50, 112, 125	0
1	F	395/424 (93%)	0.21	24 (6%) 27 29	29, 49, 107, 113	0
All	All	2433/2544 (95%)	0.08	110 (4%) 38 40	26, 47, 99, 125	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	257	LEU	5.4
1	F	269	LEU	4.8
1	A	324	ARG	4.8
1	E	269	LEU	4.6
1	E	334	THR	4.3
1	C	271	LYS	4.2
1	C	302	ALA	4.1
1	C	324	ARG	4.0
1	E	310	ALA	4.0
1	E	258	TYR	3.8
1	E	287	THR	3.7
1	E	314	HIS	3.7
1	E	263	LEU	3.7
1	E	253	ALA	3.7
1	E	265	ILE	3.5
1	C	286	ILE	3.4
1	F	304	ILE	3.4
1	D	324	ARG	3.4
1	C	287	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	302	ALA	3.2
1	F	268	LEU	3.2
1	E	291	LEU	3.2
1	E	250	ILE	3.1
1	E	232	ALA	3.0
1	F	313	ALA	3.0
1	C	248	ILE	3.0
1	F	253	ALA	3.0
1	F	331	ILE	3.0
1	E	255	GLY	2.9
1	E	93	LYS	2.9
1	E	324	ARG	2.9
1	F	286	ILE	2.9
1	E	299	LEU	2.8
1	C	275	PHE	2.8
1	C	278	VAL	2.8
1	D	334	THR	2.8
1	D	277	MET	2.8
1	C	265	ILE	2.8
1	C	93	LYS	2.8
1	D	302	ALA	2.8
1	E	308	ILE	2.7
1	C	277	MET	2.7
1	B	324	ARG	2.7
1	E	333	ALA	2.7
1	E	295	ASP	2.6
1	C	325	ALA	2.6
1	F	267	TYR	2.6
1	E	268	LEU	2.6
1	D	253	ALA	2.6
1	F	314	HIS	2.6
1	E	100	TRP	2.6
1	A	275	PHE	2.6
1	E	248	ILE	2.6
1	E	267	TYR	2.6
1	E	313	ALA	2.5
1	E	266	PRO	2.5
1	C	250	ILE	2.5
1	C	312	ASN	2.5
1	E	303	ALA	2.5
1	F	310	ALA	2.5
1	E	260	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	222	ALA	2.5
1	C	279	THR	2.4
1	E	329	THR	2.4
1	E	292	LEU	2.4
1	E	243	ALA	2.3
1	E	264	ASP	2.3
1	C	314	HIS	2.3
1	E	256	GLY	2.3
1	F	303	ALA	2.3
1	C	319	SER	2.3
1	F	15	LEU	2.3
1	F	338	ASN	2.3
1	D	303	ALA	2.3
1	C	220	GLN	2.3
1	E	217	ILE	2.3
1	C	268	LEU	2.2
1	E	236	LEU	2.2
1	F	257	LEU	2.2
1	C	252	ASP	2.2
1	F	324	ARG	2.2
1	C	219	LEU	2.2
1	C	285	VAL	2.2
1	F	229	PHE	2.2
1	B	284	ASP	2.2
1	C	276	GLY	2.2
1	C	241	HIS	2.2
1	F	93	LYS	2.2
1	C	224	ILE	2.2
1	C	263	LEU	2.2
1	D	344	LEU	2.2
1	C	221	ASN	2.2
1	C	260	PRO	2.2
1	C	303	ALA	2.2
1	D	245	ALA	2.2
1	F	266	PRO	2.2
1	F	291	LEU	2.1
1	E	251	SER	2.1
1	F	336	ILE	2.1
1	A	254	ASN	2.1
1	F	247	VAL	2.1
1	C	222	ALA	2.1
1	E	312	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	247	VAL	2.1
1	F	226	ILE	2.0
1	C	321	VAL	2.0
1	C	309	THR	2.0
1	A	236	LEU	2.0
1	C	281	LEU	2.0
1	F	260	PRO	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	C	425	7/7	0.87	0.12	54,56,60,64	0
2	PEG	E	425	7/7	0.89	0.14	59,60,65,65	0
2	PEG	D	425	7/7	0.90	0.10	51,52,56,56	0
2	PEG	A	425	7/7	0.93	0.14	44,49,57,58	0
2	PEG	F	425	7/7	0.93	0.09	44,45,51,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.