Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 02:15 PM EST

PDB ID	:	3K92
Title	:	Crystal structure of a E93K mutant of the majour 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:

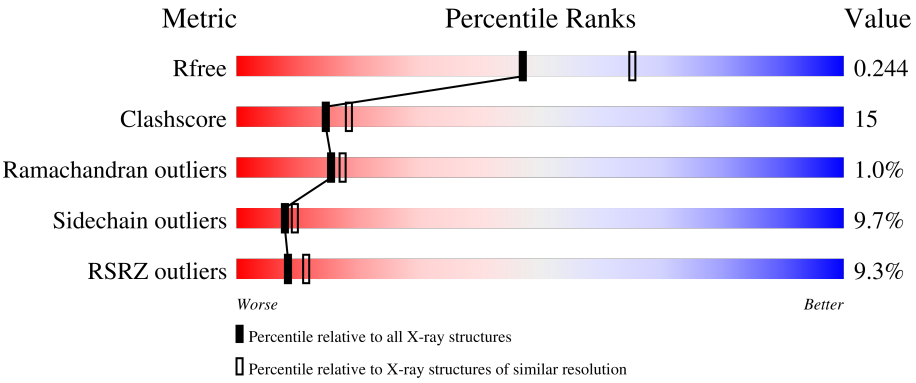
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	2% 73% 20% 6%
1	B	424	3% 71% 19% 6%
1	C	424	14% 69% 21% 6%
1	D	424	7% 71% 20% 5%
1	E	424	15% 62% 25% 6% 7%

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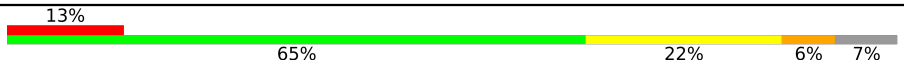
Mol	Chain	Length	Quality of chain
1	F	424	

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 (i)

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.

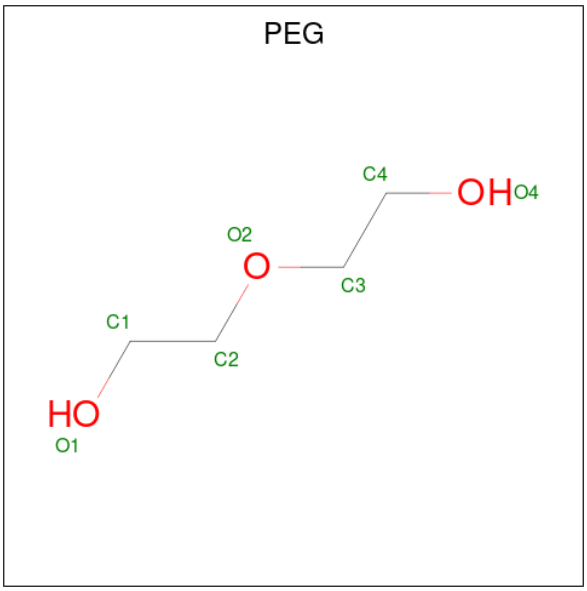
- Molecule 1 is a protein called NAD-specific glutamate dehydrogenase.

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 (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 3 is water.

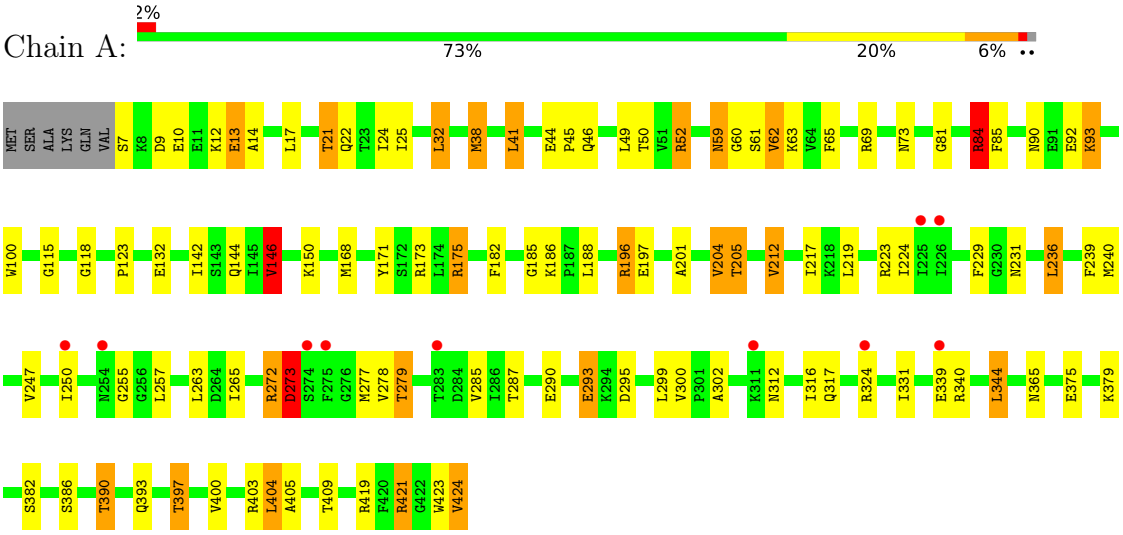
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	187	Total O 187 187	0	0
3	B	161	Total O 161 161	0	0
3	C	133	Total O 133 133	0	0
3	D	112	Total O 112 112	0	0
3	E	108	Total O 108 108	0	0
3	F	123	Total O 123 123	0	0

3 Residue-property plots (i)

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

Chain A:

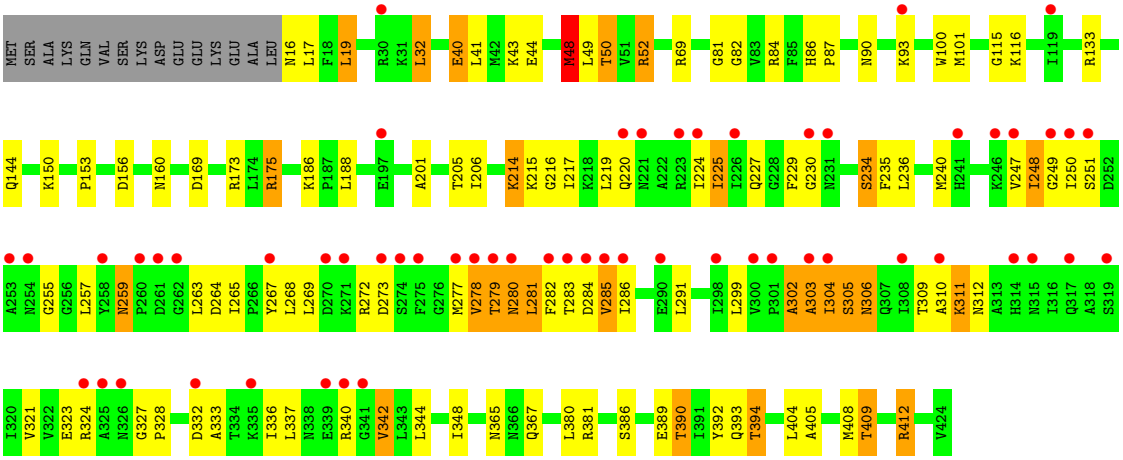


• Molecule 1: NAD-specific glutamate dehydrogenase

Chain B:

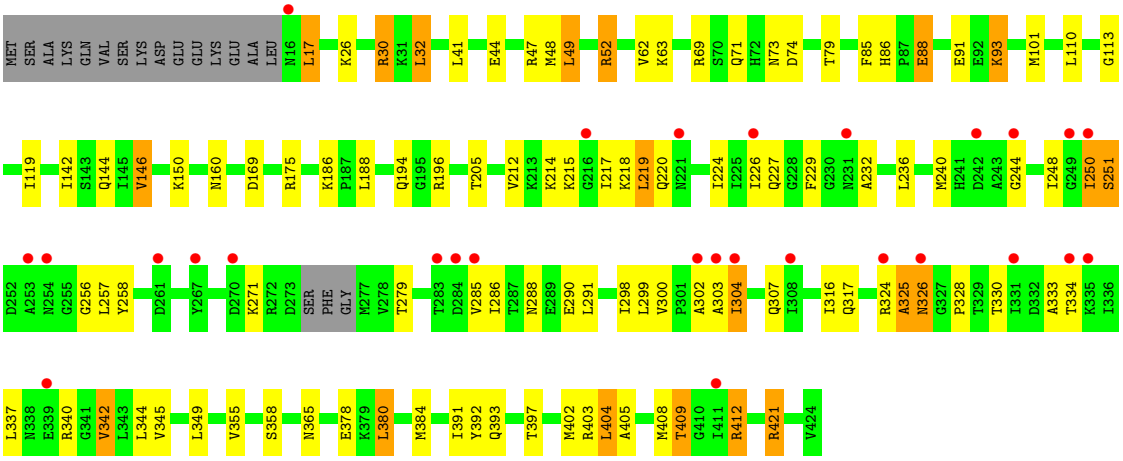
• Molecule 1: NAD-specific glutamate dehydrogenase

Chain C:



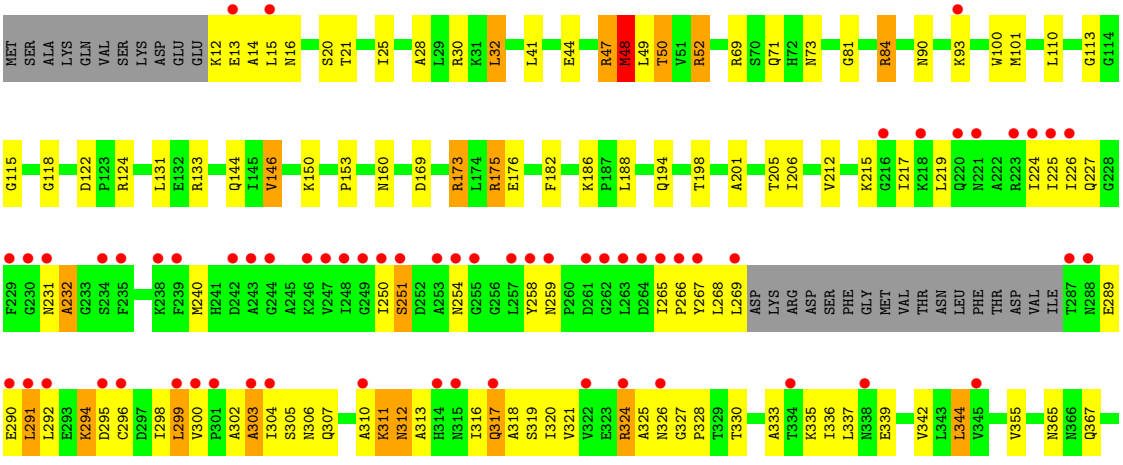
• Molecule 1: NAD-specific glutamate dehydrogenase

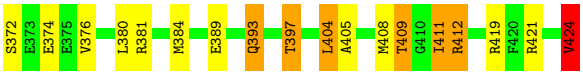
Chain D:



• Molecule 1: NAD-specific glutamate dehydrogenase

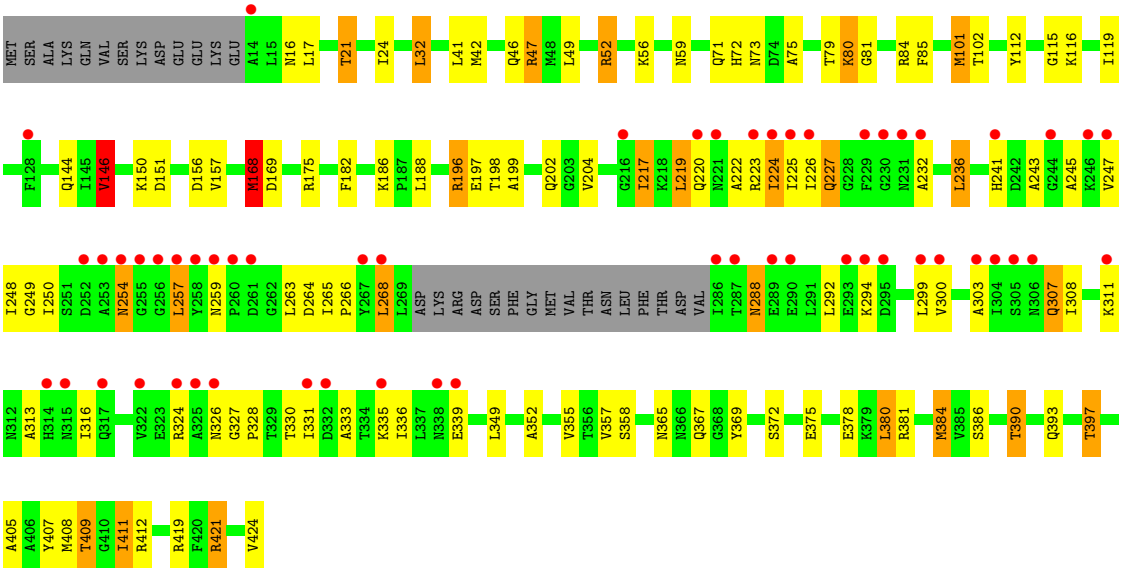
Chain E:





• Molecule 1: NAD-specific glutamate dehydrogenase

Chain F:



4 Data and refinement statistics (i)

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 18.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (18.67-2.30) 99.8 (18.64-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.238 0.189 , 0.244	Depositor DCC
R_{free} test set	7159 reflections (5.04%)	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)	0.36 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.12	5/3289 (0.2%)	1.10	20/4443 (0.5%)
1	B	1.09	5/3217 (0.2%)	1.12	14/4348 (0.3%)
1	C	1.00	1/3217 (0.0%)	0.97	11/4348 (0.3%)
1	D	0.96	1/3186 (0.0%)	0.93	9/4306 (0.2%)
1	E	1.01	0/3107	1.05	17/4197 (0.4%)
1	F	1.00	2/3099 (0.1%)	0.97	14/4188 (0.3%)
All	All	1.03	14/19115 (0.1%)	1.03	85/25830 (0.3%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	LYS	CE-NZ	6.78	1.66	1.49
1	B	374	GLU	CG-CD	5.97	1.60	1.51
1	B	27	GLU	CG-CD	5.81	1.60	1.51
1	B	375	GLU	CB-CG	5.66	1.62	1.52
1	C	40	GLU	CB-CG	5.65	1.62	1.52
1	B	75	ALA	CA-CB	5.61	1.64	1.52
1	A	421	ARG	CD-NE	-5.59	1.36	1.46
1	F	75	ALA	CA-CB	5.46	1.64	1.52
1	A	13	GLU	CG-CD	5.43	1.60	1.51
1	A	375	GLU	CG-CD	5.19	1.59	1.51
1	F	196	ARG	CZ-NH1	5.16	1.39	1.33
1	D	378	GLU	CG-CD	5.16	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	VAL	CB-CG2	5.11	1.63	1.52
1	A	339	GLU	CG-CD	5.03	1.59	1.51

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	133	ARG	NE-CZ-NH2	-18.35	111.12	120.30
1	B	175	ARG	NE-CZ-NH1	15.37	127.98	120.30
1	E	47	ARG	NE-CZ-NH2	-14.57	113.01	120.30
1	E	133	ARG	NE-CZ-NH2	-14.01	113.30	120.30
1	C	133	ARG	NE-CZ-NH2	-13.97	113.32	120.30
1	A	52	ARG	NE-CZ-NH2	-13.81	113.39	120.30
1	B	175	ARG	NE-CZ-NH2	-13.61	113.50	120.30
1	E	175	ARG	NE-CZ-NH1	12.39	126.50	120.30
1	B	133	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	E	175	ARG	NE-CZ-NH2	-11.87	114.37	120.30
1	C	175	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	E	47	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	C	133	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	A	175	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	C	175	ARG	NE-CZ-NH2	-9.81	115.40	120.30
1	B	47	ARG	NE-CZ-NH2	-9.75	115.43	120.30
1	F	47	ARG	NE-CZ-NH1	9.45	125.02	120.30
1	E	133	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	B	52	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	F	196	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	D	52	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	52	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	F	52	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	A	421	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	D	52	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	A	175	ARG	NE-CZ-NH2	-8.47	116.07	120.30
1	B	47	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	A	196	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	A	146	VAL	CG1-CB-CG2	8.12	123.89	110.90
1	B	421	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	F	47	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	C	101	MET	CG-SD-CE	-8.00	87.39	100.20
1	F	168	MET	CG-SD-CE	7.84	112.75	100.20
1	B	52	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	421	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	E	52	ARG	NE-CZ-NH1	6.93	123.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	101	MET	CG-SD-CE	-6.84	89.26	100.20
1	A	403	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	F	196	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	F	52	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	D	175	ARG	NE-CZ-NH2	6.65	123.62	120.30
1	C	52	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	340	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	B	133	ARG	CG-CD-NE	-6.53	98.09	111.80
1	B	175	ARG	CD-NE-CZ	6.52	132.72	123.60
1	A	69	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	C	32	LEU	CA-CB-CG	6.24	129.66	115.30
1	A	340	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	32	LEU	CA-CB-CG	6.07	129.27	115.30
1	E	133	ARG	CG-CD-NE	-6.05	99.09	111.80
1	E	175	ARG	CD-NE-CZ	6.00	132.00	123.60
1	A	295	ASP	CB-CG-OD1	5.98	123.68	118.30
1	F	411	ILE	CB-CA-C	-5.88	99.83	111.60
1	A	84	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	44	GLU	CA-CB-CG	5.74	126.02	113.40
1	A	196	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	E	324	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	F	421	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	E	421	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	D	146	VAL	CG1-CB-CG2	5.59	119.84	110.90
1	B	421	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	D	196	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	403	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	D	196	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	E	69	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	E	424	VAL	CB-CA-C	-5.40	101.13	111.40
1	E	101	MET	CG-SD-CE	-5.37	91.61	100.20
1	F	175	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	F	424	VAL	CB-CA-C	-5.35	101.24	111.40
1	C	69	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	273	ASP	CB-CA-C	-5.34	99.73	110.40
1	C	412	ARG	CG-CD-NE	-5.32	100.64	111.80
1	F	412	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	344	LEU	CA-CB-CG	5.30	127.50	115.30
1	D	69	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	D	412	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	E	52	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	F	146	VAL	CG1-CB-CG2	5.15	119.13	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	223	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	48	MET	CG-SD-CE	-5.12	92.01	100.20
1	E	412	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	44	GLU	N-CA-CB	-5.11	101.41	110.60
1	C	133	ARG	CG-CD-NE	-5.03	101.24	111.80
1	E	48	MET	CG-SD-CE	-5.01	92.19	100.20
1	D	421	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	101	0
1	B	3158	0	3179	91	0
1	C	3158	0	3179	107	0
1	D	3129	0	3145	95	0
1	E	3051	0	3075	113	0
1	F	3043	0	3072	105	0
2	A	7	0	10	0	0
2	C	7	0	10	3	0
2	D	7	0	10	4	0
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	5	0
3	F	123	0	0	7	0
All	All	19628	0	18948	579	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 15.

All (579) 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:A:38:MET:HE3	1:A:38:MET:HA	1.43	0.98
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:62:VAL:HG21	1:B:424:VAL:HG12	1.67	0.74
1:B:59:ASN:C	1:B:59:ASN:HD22	1.91	0.74
1:F:219:LEU:CD1	1:F:243:ALA:HB1	2.15	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
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: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: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:B:42:MET:HE2	1:B:72:HIS:CE1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:32:LEU:HD13	1:E:408:MET:HE2	1.73	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:D:32:LEU:HD13	1:D:408:MET:HE3	1.75	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:F:101:MET:HE1	3:F:503:HOH:O	1.94	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
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:A:132:GLU:OE2	3:A:517:HOH:O	2.13	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:THR:HG22	1:D:236:LEU:HD13	1.79	0.65
1:A:150:LYS:HZ3	1:B:144:GLN:HE21	1.45	0.64
1:D:32:LEU:HD13	1:D:408:MET:CE	2.26	0.64
1:F:32:LEU:HD13	1:F:408:MET:HE3	1.79	0.64
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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:146:VAL:HG13	1:B:182:PHE:HE1	1.65	0.60
1:C:48:MET:HE1	1:C:50:THR:HG22	1.84	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: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:E:319:SER:C	1:E:342:VAL:HG23	2.23	0.59
1:A:255:GLY:HA3	1:A:285:VAL:HG13	1.84	0.59
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:227:GLN:C	1:E:302:ALA:HB2	2.23	0.58
1:E:393:GLN:O	1:E:397:THR:CG2	2.51	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:A:38:MET:HA	1:A:38:MET:CE	2.28	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:E:224:ILE:HG21	1:E:240:MET:HG3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:THR:HG22	1:D:236:LEU:CD1	2.34	0.57
1:E:268:LEU:C	1:E:269:LEU:HD22	2.24	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: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:E:295:ASP:CB	1:E:317:GLN:NE2	2.68	0.56
1:E:48:MET:HE1	1:E:50:THR:HG22	1.87	0.56
1:B:390:THR:O	1:B:394:THR:CG2	2.52	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
1:D:219:LEU:CD2	1:D:240:MET:HE3	2.36	0.56
1:F:42:MET:HE2	1:F:72:HIS:CE1	2.41	0.56
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:C:48:MET:CE	1:C:50:THR:HG22	2.36	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: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:B:90:ASN:C	1:B:90:ASN:HD22	2.08	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: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:59:ASN:C	1:B:59:ASN:ND2	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:THR:OG1	1:B:334:THR:HG22	2.06	0.54
1:E:169:ASP:HB2	1:F:421:ARG:HD3	1.90	0.54
1:E:335:LYS:NZ	1:E:339:GLU:OE2	2.40	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
1:D:150:LYS:HZ2	1:E:144:GLN:HE21	1.54	0.54
3:C:437:HOH:O	1:F:52:ARG:HD3	2.08	0.53
1:D:144:GLN:HE21	1:E:150:LYS:HZ3	1.55	0.53
1:D:160:ASN:ND2	2:D:425:PEG:H21	2.21	0.53
1:E:160:ASN:HD21	2:E:425:PEG:H22	1.72	0.53
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:A:59:ASN:C	1:A:59:ASN:HD22	2.10	0.53
1:B:214:LYS:HG2	1:B:392:TYR:CZ	2.44	0.53
1:E:48:MET:CE	1:E:50:THR:HG22	2.38	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: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:C:303:ALA:C	1:C:304:ILE:HD13	2.30	0.53
1:E:311:LYS:O	1:E:312:ASN:CG	2.47	0.53
1:B:345:VAL:HA	1:B:402:MET:HE3	1.90	0.52
1:D:186:LYS:NZ	1:D:365:ASN:HD21	2.06	0.52
1:B:42:MET:HE3	1:B:42:MET:HA	1.90	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:38:MET:HE1	1:A:41:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LYS:HE2	1:F:369:TYR:OH	2.10	0.52
1:B:218:LYS:NZ	3:B:586:HOH:O	2.43	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: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: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:B:419:ARG:C	1:B:419:ARG:HD2	2.30	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
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:F:349:LEU:HD11	1:F:384:MET:HE1	1.93	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:C:186:LYS:NZ	1:C:365:ASN:HD21	2.10	0.50
3:D:470:HOH:O	1:E:52:ARG:HD3	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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: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:A:38:MET:HE3	1:A:38:MET:CA	2.31	0.47
1:A:38:MET:HE3	1:A:424:VAL:HG21	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:169:ASP:OD1	1:D:421:ARG:HD2	2.15	0.47
1:C:284:ASP:O	1:C:285:VAL:HG23	2.15	0.47
1:D:48:MET:HE2	1:D:91:GLU:HG3	1.97	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:F:59:ASN:C	1:F:59:ASN:OD1	2.52	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:D:219:LEU:HD23	1:D:240:MET:HE3	1.96	0.47
1:E:81:GLY:O	1:E:153:PRO:HA	2.14	0.47
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: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:F:42:MET:HE3	1:F:72:HIS:CE1	2.50	0.46
1:C:278:VAL:HG12	1:C:279:THR:N	2.28	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:C:227:GLN:HA	1:C:251:SER:HB3	1.98	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:A:196:ARG:HG2	1:A:197:GLU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ILE:HD13	1:C:240:MET:HG3	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
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:D:344:LEU:C	1:D:344:LEU:HD23	2.36	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:311:LYS:O	1:E:312:ASN:CB	2.64	0.45
1:A:59:ASN:C	1:A:59:ASN:ND2	2.69	0.45
1:C:100:TRP:HZ3	1:C:348:ILE:HD12	1.80	0.45
1:D:279:THR:HG23	1:D:285:VAL:CG2	2.46	0.45
1:F:196:ARG:HD2	3:F:634:HOH:O	2.16	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: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:160:ASN:HD21	2:E:425:PEG:H21	1.81	0.45
1:A:150:LYS:HZ2	1:B:144:GLN:HE21	1.57	0.44
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:C:82:GLY:O	1:C:116:LYS:HD3	2.18	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:305:SER:O	1:E:307:GLN:HG3	2.18	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:F:384:MET:HE3	1:F:384:MET:HA	2.00	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:F:224:ILE:HG22	1:F:247:VAL:HA	1.99	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:110:LEU:HD11	1:E:355:VAL:CG1	2.45	0.43
1:F:42:MET:HE1	1:F:72:HIS:CE1	2.52	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:D:345:VAL:HG22	1:D:402:MET:HE1	2.00	0.43
1:B:343:LEU:HD11	1:B:402:MET:CE	2.48	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
1:B:84:ARG:CG	1:B:156:ASP:OD1	2.67	0.43
1:C:90:ASN:ND2	1:C:93:LYS:HE3	2.14	0.43
1:F:259:ASN:HB3	1:F:263:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ASN:N	1:C:19:LEU:HD22	2.29	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:B:90:ASN:HD21	1:B:93:LYS:HG3	1.84	0.42
1:F:42:MET:HE3	1:F:72:HIS:NE2	2.35	0.42
1:B:412:ARG:CG	1:B:416:GLU:OE2	2.67	0.42
1:C:144:GLN:HE21	1:F:150:LYS:HZ3	1.68	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:D:32:LEU:CD1	1:D:408:MET:HE2	2.50	0.42
1:D:186:LYS:HZ1	1:D:365:ASN:HD21	1.67	0.42
1:E:48:MET:HB3	1:E:48:MET:HE2	1.80	0.42
1:E:268:LEU:O	1:E:269:LEU:HD13	2.19	0.42
1:F:168:MET:HE3	1:F:169:ASP:HA	2.00	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:E:268:LEU:O	1:E:269:LEU:HD22	2.19	0.42
1:A:144:GLN:HE21	1:B:150:LYS:HZ2	1.66	0.42
1:B:325:ALA:HA	1:B:347:ASP:OD1	2.19	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:168:MET:HE3	1:B:169:ASP:HA	2.01	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:C:44:GLU:HB2	1:F:52:ARG:CD	2.46	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:186:LYS:HZ2	1:A:365:ASN:HD21	1.67	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:F:249:GLY:C	1:F:250:ILE:HD12	2.41	0.41
1:B:345:VAL:HG22	1:B:402:MET:CE	2.51	0.41
1:C:186:LYS:HZ2	1:C:365:ASN:HD21	1.67	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:D:48:MET:CE	1:D:91:GLU:HG3	2.51	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:256:GLY:C	1:D:257:LEU:HD22	2.42	0.41
1:F:80:LYS:CG	1:F:112:TYR:CE2	3.04	0.41
1:F:101:MET:O	1:F:102:THR:C	2.60	0.41
1:C:50:THR:HG23	3:F:430:HOH:O	2.21	0.40
1:C:186:LYS:HZ2	1:C:365:ASN:ND2	2.19	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:254:ASN:N	1:F:254:ASN:ND2	2.66	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
1:A:272:ARG:HD2	3:A:536:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:F:42:MET:CE	1:F:72:HIS:HE1	2.30	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%)	22	26
1	B	407/424 (96%)	396 (97%)	10 (2%)	1 (0%)	47	58
1	C	407/424 (96%)	376 (92%)	19 (5%)	12 (3%)	4	3
1	D	402/424 (95%)	383 (95%)	17 (4%)	2 (0%)	29	35
1	E	392/424 (92%)	360 (92%)	27 (7%)	5 (1%)	12	12
1	F	391/424 (92%)	367 (94%)	22 (6%)	2 (0%)	29	35
All	All	2415/2544 (95%)	2282 (94%)	108 (4%)	25 (1%)	15	17

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	ASP
1	C	248	ILE
1	C	283	THR

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	346/351 (99%)	311 (90%)	35 (10%)	7 9
1	B	338/351 (96%)	305 (90%)	33 (10%)	8 9
1	C	338/351 (96%)	306 (90%)	32 (10%)	8 10
1	D	333/351 (95%)	311 (93%)	22 (7%)	16 22
1	E	324/351 (92%)	288 (89%)	36 (11%)	6 7
1	F	324/351 (92%)	287 (89%)	37 (11%)	5 6
All	All	2003/2106 (95%)	1808 (90%)	195 (10%)	8 9

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	12	LYS
1	A	13	GLU
1	A	21	THR
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	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	231	ASN
1	A	236	LEU
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	419	ARG
1	A	424	VAL
1	B	17	LEU
1	B	21	THR
1	B	32	LEU
1	B	41	LEU
1	B	49	LEU
1	B	50	THR
1	B	56	LYS

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Mol	Chain	Res	Type
1	B	59	ASN
1	B	90	ASN
1	B	146	VAL
1	B	168	MET
1	B	173	ARG
1	B	188	LEU
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	326	ASN
1	B	329	THR
1	B	334	THR
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
1	C	49	LEU
1	C	50	THR
1	C	52	ARG
1	C	188	LEU
1	C	214	LYS
1	C	219	LEU
1	C	220	GLN
1	C	225	ILE
1	C	229	PHE
1	C	234	SER
1	C	236	LEU

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Mol	Chain	Res	Type
1	C	267	TYR
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	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	88	GLU
1	D	93	LYS
1	D	146	VAL
1	D	188	LEU
1	D	215	LYS
1	D	219	LEU
1	D	250	ILE
1	D	251	SER
1	D	271	LYS
1	D	299	LEU
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	E	12	LYS
1	E	13	GLU
1	E	15	LEU
1	E	30	ARG

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Mol	Chain	Res	Type
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	100	TRP
1	E	146	VAL
1	E	173	ARG
1	E	188	LEU
1	E	219	LEU
1	E	231	ASN
1	E	251	SER
1	E	254	ASN
1	E	267	TYR
1	E	291	LEU
1	E	294	LYS
1	E	299	LEU
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	32	LEU
1	F	41	LEU
1	F	49	LEU
1	F	56	LYS
1	F	80	LYS
1	F	84	ARG
1	F	146	VAL
1	F	168	MET

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Mol	Chain	Res	Type
1	F	188	LEU
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	227	GLN
1	F	236	LEU
1	F	248	ILE
1	F	254	ASN
1	F	257	LEU
1	F	288	ASN
1	F	299	LEU
1	F	307	GLN
1	F	311	LYS
1	F	316	ILE
1	F	326	ASN
1	F	358	SER
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	409	THR
1	F	411	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) 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	312	ASN
1	A	365	ASN
1	A	367	GLN
1	A	393	GLN
1	B	59	ASN
1	B	90	ASN

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Mol	Chain	Res	Type
1	B	144	GLN
1	B	194	GLN
1	B	202	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	365	ASN
1	B	367	GLN
1	B	393	GLN
1	C	90	ASN
1	C	144	GLN
1	C	162	GLN
1	C	194	GLN
1	C	202	GLN
1	C	288	ASN
1	C	312	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	194	GLN
1	E	254	ASN
1	E	259	ASN
1	E	312	ASN
1	E	317	GLN
1	E	365	ASN

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Mol	Chain	Res	Type
1	E	367	GLN
1	F	144	GLN
1	F	202	GLN
1	F	220	GLN
1	F	221	ASN
1	F	227	GLN
1	F	241	HIS
1	F	254	ASN
1	F	288	ASN
1	F	326	ASN
1	F	365	ASN
1	F	393	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	D	425	-	6,6,6	0.52	0	5,5,5	0.54	0
2	PEG	A	425	-	6,6,6	0.51	0	5,5,5	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PEG	F	425	-	6,6,6	0.41	0	5,5,5	0.32	0
2	PEG	E	425	-	6,6,6	0.67	0	5,5,5	0.49	0
2	PEG	C	425	-	6,6,6	0.38	0	5,5,5	0.78	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	D	425	-	-	3/4/4/4	-
2	PEG	A	425	-	-	2/4/4/4	-
2	PEG	F	425	-	-	1/4/4/4	-
2	PEG	E	425	-	-	2/4/4/4	-
2	PEG	C	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	E	425	PEG	4	0
2	C	425	PEG	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.12	10 (2%) 59 66	26, 40, 64, 80	0
1	B	409/424 (96%)	-0.05	12 (2%) 51 58	27, 44, 69, 82	0
1	C	409/424 (96%)	0.40	58 (14%) 2 3	30, 48, 104, 114	0
1	D	406/424 (95%)	0.19	28 (6%) 16 22	29, 51, 83, 99	0
1	E	396/424 (93%)	0.48	63 (15%) 1 2	30, 50, 112, 125	0
1	F	395/424 (93%)	0.41	55 (13%) 2 4	29, 49, 107, 113	0
All	All	2433/2544 (95%)	0.21	226 (9%) 8 11	26, 47, 99, 125	0

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	267	TYR	9.0
1	E	267	TYR	8.0
1	F	303	ALA	7.6
1	F	304	ILE	6.6
1	F	226	ILE	5.8
1	E	258	TYR	5.7
1	C	283	THR	5.5
1	F	261	ASP	5.4
1	F	231	ASN	5.4
1	C	275	PHE	5.4
1	F	253	ALA	5.3
1	C	250	ILE	5.2
1	F	254	ASN	5.2
1	E	231	ASN	5.1
1	F	268	LEU	5.1
1	D	303	ALA	5.0
1	F	324	ARG	4.9
1	F	246	LYS	4.8
1	E	254	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	306	ASN	4.7
1	D	285	VAL	4.7
1	E	257	LEU	4.7
1	C	324	ARG	4.7
1	B	283	THR	4.6
1	C	284	ASP	4.6
1	E	261	ASP	4.6
1	A	275	PHE	4.4
1	F	335	LYS	4.4
1	E	295	ASP	4.3
1	E	299	LEU	4.3
1	D	308	ILE	4.2
1	F	339	GLU	4.1
1	F	260	PRO	4.1
1	E	287	THR	4.1
1	D	324	ARG	4.1
1	F	224	ILE	4.1
1	C	246	LYS	4.1
1	E	263	LEU	4.0
1	C	303	ALA	4.0
1	E	303	ALA	4.0
1	C	274	SER	4.0
1	C	304	ILE	4.0
1	C	260	PRO	4.0
1	E	324	ARG	3.9
1	D	231	ASN	3.9
1	C	220	GLN	3.9
1	E	253	ALA	3.9
1	F	287	THR	3.9
1	C	221	ASN	3.8
1	E	266	PRO	3.8
1	E	290	GLU	3.7
1	C	280	ASN	3.7
1	F	252	ASP	3.7
1	F	229	PHE	3.7
1	E	314	HIS	3.7
1	C	226	ILE	3.7
1	C	261	ASP	3.6
1	C	267	TYR	3.6
1	F	247	VAL	3.6
1	F	225	ILE	3.6
1	B	284	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	232	ALA	3.6
1	C	286	ILE	3.5
1	A	274	SER	3.5
1	A	311	LYS	3.5
1	C	241	HIS	3.5
1	C	314	HIS	3.5
1	E	315	ASN	3.5
1	D	226	ILE	3.5
1	F	314	HIS	3.5
1	E	226	ILE	3.5
1	E	264	ASP	3.5
1	F	326	ASN	3.4
1	C	273	ASP	3.4
1	C	308	ILE	3.4
1	C	231	ASN	3.4
1	E	220	GLN	3.3
1	C	254	ASN	3.3
1	F	331	ILE	3.3
1	F	14	ALA	3.3
1	E	243	ALA	3.3
1	C	335	LYS	3.2
1	E	304	ILE	3.2
1	E	247	VAL	3.2
1	D	253	ALA	3.2
1	E	224	ILE	3.2
1	E	310	ALA	3.2
1	E	262	GLY	3.2
1	E	216	GLY	3.2
1	C	278	VAL	3.1
1	B	324	ARG	3.1
1	C	277	MET	3.1
1	E	255	GLY	3.1
1	E	265	ILE	3.1
1	E	288	ASN	3.1
1	F	290	GLU	3.1
1	D	261	ASP	3.1
1	D	270	ASP	3.1
1	F	294	LYS	3.1
1	F	317	GLN	3.1
1	F	286	ILE	3.1
1	F	221	ASN	3.0
1	F	259	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	332	ASP	3.0
1	D	254	ASN	3.0
1	C	285	VAL	3.0
1	E	242	ASP	3.0
1	D	267	TYR	3.0
1	E	218	LYS	3.0
1	B	303	ALA	3.0
1	F	230	GLY	3.0
1	C	315	ASN	2.9
1	C	339	GLU	2.9
1	D	242	ASP	2.9
1	D	331	ILE	2.9
1	E	229	PHE	2.9
1	D	339	GLU	2.9
1	F	325	ALA	2.9
1	E	225	ILE	2.9
1	C	279	THR	2.9
1	F	257	LEU	2.9
1	F	258	TYR	2.9
1	C	93	LYS	2.8
1	E	251	SER	2.8
1	E	334	THR	2.8
1	F	305	SER	2.8
1	E	15	LEU	2.8
1	E	223	ARG	2.8
1	D	304	ILE	2.8
1	C	290	GLU	2.8
1	C	262	GLY	2.7
1	C	319	SER	2.7
1	A	283	THR	2.7
1	D	221	ASN	2.7
1	D	326	ASN	2.7
1	E	326	ASN	2.7
1	E	93	LYS	2.7
1	E	317	GLN	2.7
1	F	256	GLY	2.7
1	D	334	THR	2.7
1	E	338	ASN	2.7
1	F	311	LYS	2.6
1	E	250	ILE	2.6
1	C	340	ARG	2.6
1	D	216	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	326	ASN	2.6
1	C	247	VAL	2.6
1	E	246	LYS	2.6
1	E	248	ILE	2.6
1	E	291	LEU	2.5
1	A	254	ASN	2.5
1	E	244	GLY	2.5
1	C	270	ASP	2.5
1	E	13	GLU	2.5
1	F	299	LEU	2.5
1	C	301	PRO	2.5
1	E	221	ASN	2.5
1	C	119	ILE	2.5
1	C	332	ASP	2.5
1	E	269	LEU	2.5
1	F	295	ASP	2.4
1	A	339	GLU	2.4
1	B	311	LYS	2.4
1	D	302	ALA	2.4
1	D	284	ASP	2.4
1	D	411	ILE	2.4
1	F	255	GLY	2.4
1	E	238	LYS	2.4
1	B	308	ILE	2.4
1	D	250	ILE	2.4
1	C	341	GLY	2.4
1	C	271	LYS	2.4
1	D	249	GLY	2.4
1	D	283	THR	2.3
1	C	282	PHE	2.3
1	F	338	ASN	2.3
1	E	300	VAL	2.3
1	E	322	VAL	2.3
1	C	251	SER	2.3
1	E	249	GLY	2.3
1	C	325	ALA	2.3
1	E	292	LEU	2.3
1	E	239	PHE	2.3
1	A	250	ILE	2.3
1	C	258	TYR	2.3
1	E	296	CYS	2.3
1	F	216	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	324	ARG	2.2
1	C	197	GLU	2.2
1	C	223	ARG	2.2
1	F	244	GLY	2.2
1	F	300	VAL	2.2
1	D	244	GLY	2.2
1	C	249	GLY	2.2
1	F	289	GLU	2.2
1	E	235	PHE	2.2
1	B	16	ASN	2.2
1	A	225	ILE	2.2
1	C	326	ASN	2.1
1	D	335	LYS	2.1
1	B	281	LEU	2.1
1	E	259	ASN	2.1
1	F	241	HIS	2.1
1	B	331	ILE	2.1
1	F	220	GLN	2.1
1	E	301	PRO	2.1
1	C	230	GLY	2.1
1	C	224	ILE	2.1
1	E	230	GLY	2.1
1	F	322	VAL	2.1
1	B	231	ASN	2.1
1	E	345	VAL	2.1
1	B	275	PHE	2.1
1	F	223	ARG	2.1
1	E	234	SER	2.1
1	C	317	GLN	2.0
1	A	226	ILE	2.0
1	C	298	ILE	2.0
1	C	310	ALA	2.0
1	F	128	PHE	2.0
1	D	16	ASN	2.0
1	C	300	VAL	2.0
1	F	315	ASN	2.0
1	F	293	GLU	2.0
1	C	30	ARG	2.0
1	C	253	ALA	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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
2	PEG	C	425	7/7	0.87	0.17	54,56,60,64	0
2	PEG	F	425	7/7	0.88	0.16	44,45,51,59	0
2	PEG	E	425	7/7	0.89	0.14	59,60,65,65	0
2	PEG	A	425	7/7	0.91	0.15	44,49,57,58	0
2	PEG	D	425	7/7	0.92	0.11	51,52,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.