



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:01 PM UTC

PDB ID : 3A11 / pdb_00003a11
Title : Crystal structure of ribose-1,5-bisphosphate isomerase from *Thermococcus kodakaraensis* KOD1
Authors : Nakamura, A.; Fujihashi, M.; Nishiba, Y.; Yoshida, S.; Yano, A.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on : 2009-03-25
Resolution : 2.50 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

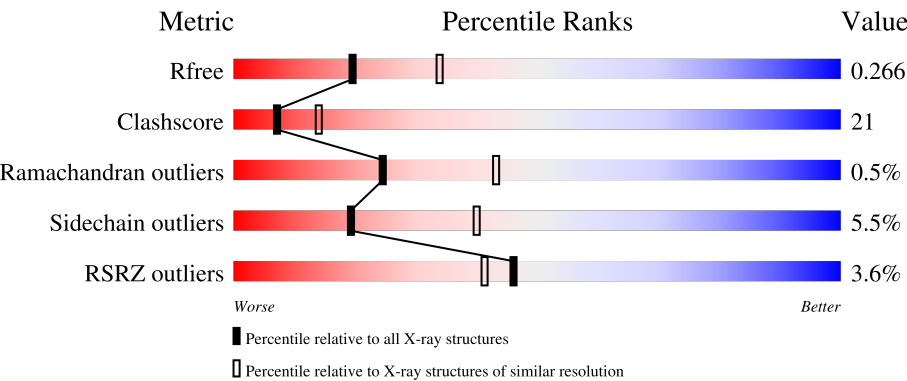
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	338	4% 62% 28% 5% 5%
1	B	338	% 62% 29% 5% 5%
1	C	338	8% 57% 33% • 6%
1	D	338	4% 62% 29% • 5%
1	E	338	% 63% 28% • 6%

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Mol	Chain	Length	Quality of chain
1	F	338	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '51%', a large yellow segment labeled '39%', and a small grey segment at the end labeled '6%'. The segments are separated by thin black lines.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15535 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 Translation initiation factor eIF-2B, delta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2541	1631	428	470	12			
1	B	322	Total	C	N	O	S	0	0	0
			2556	1636	435	472	13			
1	C	317	Total	C	N	O	S	0	0	0
			2513	1613	424	464	12			
1	D	320	Total	C	N	O	S	0	0	0
			2531	1623	428	468	12			
1	E	317	Total	C	N	O	S	0	0	0
			2513	1613	424	464	12			
1	F	319	Total	C	N	O	S	0	0	0
			2529	1623	426	468	12			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP Q5JFM9
A	-14	ASN	-	expression tag	UNP Q5JFM9
A	-13	HIS	-	expression tag	UNP Q5JFM9
A	-12	LYS	-	expression tag	UNP Q5JFM9
A	-11	VAL	-	expression tag	UNP Q5JFM9
A	-10	HIS	-	expression tag	UNP Q5JFM9
A	-9	HIS	-	expression tag	UNP Q5JFM9
A	-8	HIS	-	expression tag	UNP Q5JFM9
A	-7	HIS	-	expression tag	UNP Q5JFM9
A	-6	HIS	-	expression tag	UNP Q5JFM9
A	-5	HIS	-	expression tag	UNP Q5JFM9
A	-4	ILE	-	expression tag	UNP Q5JFM9
A	-3	GLU	-	expression tag	UNP Q5JFM9
A	-2	GLY	-	expression tag	UNP Q5JFM9
A	-1	ARG	-	expression tag	UNP Q5JFM9
A	0	HIS	-	expression tag	UNP Q5JFM9
B	-15	MET	-	expression tag	UNP Q5JFM9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	ASN	-	expression tag	UNP Q5JFM9
B	-13	HIS	-	expression tag	UNP Q5JFM9
B	-12	LYS	-	expression tag	UNP Q5JFM9
B	-11	VAL	-	expression tag	UNP Q5JFM9
B	-10	HIS	-	expression tag	UNP Q5JFM9
B	-9	HIS	-	expression tag	UNP Q5JFM9
B	-8	HIS	-	expression tag	UNP Q5JFM9
B	-7	HIS	-	expression tag	UNP Q5JFM9
B	-6	HIS	-	expression tag	UNP Q5JFM9
B	-5	HIS	-	expression tag	UNP Q5JFM9
B	-4	ILE	-	expression tag	UNP Q5JFM9
B	-3	GLU	-	expression tag	UNP Q5JFM9
B	-2	GLY	-	expression tag	UNP Q5JFM9
B	-1	ARG	-	expression tag	UNP Q5JFM9
B	0	HIS	-	expression tag	UNP Q5JFM9
C	-15	MET	-	expression tag	UNP Q5JFM9
C	-14	ASN	-	expression tag	UNP Q5JFM9
C	-13	HIS	-	expression tag	UNP Q5JFM9
C	-12	LYS	-	expression tag	UNP Q5JFM9
C	-11	VAL	-	expression tag	UNP Q5JFM9
C	-10	HIS	-	expression tag	UNP Q5JFM9
C	-9	HIS	-	expression tag	UNP Q5JFM9
C	-8	HIS	-	expression tag	UNP Q5JFM9
C	-7	HIS	-	expression tag	UNP Q5JFM9
C	-6	HIS	-	expression tag	UNP Q5JFM9
C	-5	HIS	-	expression tag	UNP Q5JFM9
C	-4	ILE	-	expression tag	UNP Q5JFM9
C	-3	GLU	-	expression tag	UNP Q5JFM9
C	-2	GLY	-	expression tag	UNP Q5JFM9
C	-1	ARG	-	expression tag	UNP Q5JFM9
C	0	HIS	-	expression tag	UNP Q5JFM9
D	-15	MET	-	expression tag	UNP Q5JFM9
D	-14	ASN	-	expression tag	UNP Q5JFM9
D	-13	HIS	-	expression tag	UNP Q5JFM9
D	-12	LYS	-	expression tag	UNP Q5JFM9
D	-11	VAL	-	expression tag	UNP Q5JFM9
D	-10	HIS	-	expression tag	UNP Q5JFM9
D	-9	HIS	-	expression tag	UNP Q5JFM9
D	-8	HIS	-	expression tag	UNP Q5JFM9
D	-7	HIS	-	expression tag	UNP Q5JFM9
D	-6	HIS	-	expression tag	UNP Q5JFM9
D	-5	HIS	-	expression tag	UNP Q5JFM9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ILE	-	expression tag	UNP Q5JFM9
D	-3	GLU	-	expression tag	UNP Q5JFM9
D	-2	GLY	-	expression tag	UNP Q5JFM9
D	-1	ARG	-	expression tag	UNP Q5JFM9
D	0	HIS	-	expression tag	UNP Q5JFM9
E	-15	MET	-	expression tag	UNP Q5JFM9
E	-14	ASN	-	expression tag	UNP Q5JFM9
E	-13	HIS	-	expression tag	UNP Q5JFM9
E	-12	LYS	-	expression tag	UNP Q5JFM9
E	-11	VAL	-	expression tag	UNP Q5JFM9
E	-10	HIS	-	expression tag	UNP Q5JFM9
E	-9	HIS	-	expression tag	UNP Q5JFM9
E	-8	HIS	-	expression tag	UNP Q5JFM9
E	-7	HIS	-	expression tag	UNP Q5JFM9
E	-6	HIS	-	expression tag	UNP Q5JFM9
E	-5	HIS	-	expression tag	UNP Q5JFM9
E	-4	ILE	-	expression tag	UNP Q5JFM9
E	-3	GLU	-	expression tag	UNP Q5JFM9
E	-2	GLY	-	expression tag	UNP Q5JFM9
E	-1	ARG	-	expression tag	UNP Q5JFM9
E	0	HIS	-	expression tag	UNP Q5JFM9
F	-15	MET	-	expression tag	UNP Q5JFM9
F	-14	ASN	-	expression tag	UNP Q5JFM9
F	-13	HIS	-	expression tag	UNP Q5JFM9
F	-12	LYS	-	expression tag	UNP Q5JFM9
F	-11	VAL	-	expression tag	UNP Q5JFM9
F	-10	HIS	-	expression tag	UNP Q5JFM9
F	-9	HIS	-	expression tag	UNP Q5JFM9
F	-8	HIS	-	expression tag	UNP Q5JFM9
F	-7	HIS	-	expression tag	UNP Q5JFM9
F	-6	HIS	-	expression tag	UNP Q5JFM9
F	-5	HIS	-	expression tag	UNP Q5JFM9
F	-4	ILE	-	expression tag	UNP Q5JFM9
F	-3	GLU	-	expression tag	UNP Q5JFM9
F	-2	GLY	-	expression tag	UNP Q5JFM9
F	-1	ARG	-	expression tag	UNP Q5JFM9
F	0	HIS	-	expression tag	UNP Q5JFM9

- 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	B	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		

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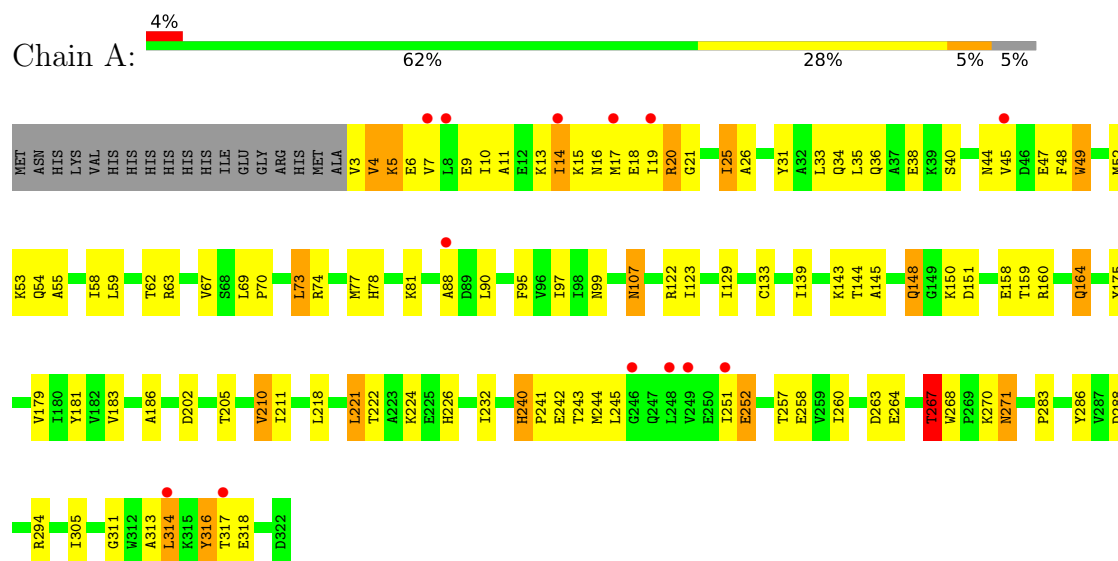
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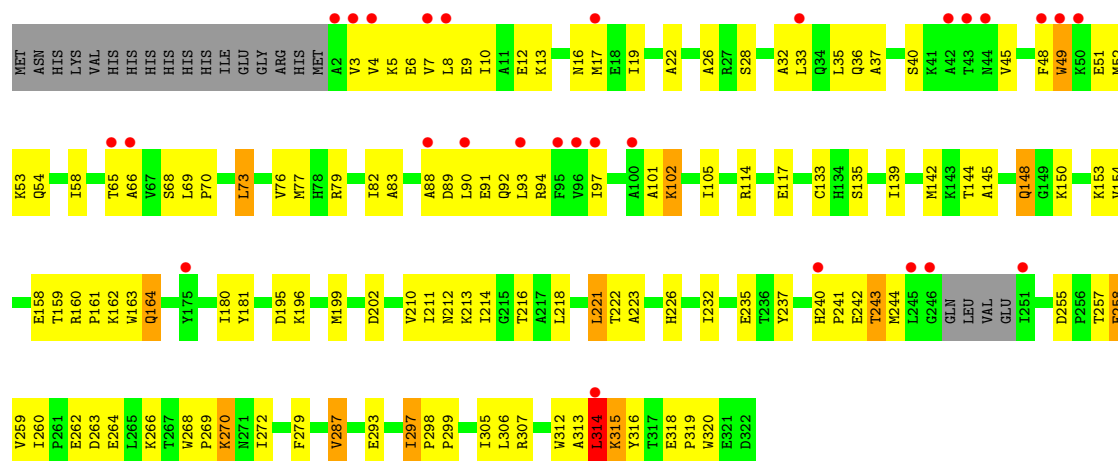
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	87	Total 87	O 87	0	0
4	C	34	Total 34	O 34	0	0
4	D	54	Total 54	O 54	0	0
4	E	46	Total 46	O 46	0	0
4	F	28	Total 28	O 28	0	0

3 Residue-property plots [i](#)

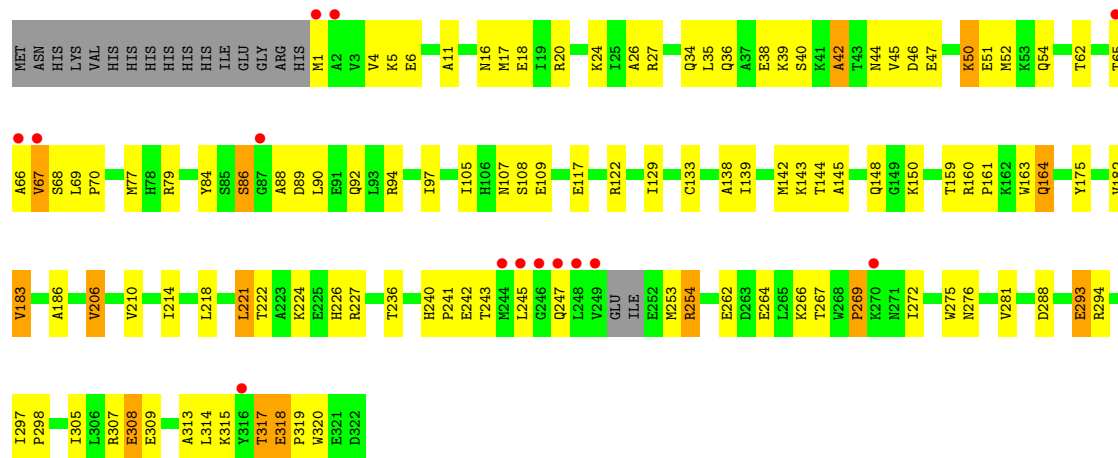
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Translation initiation factor eIF-2B, delta subunit

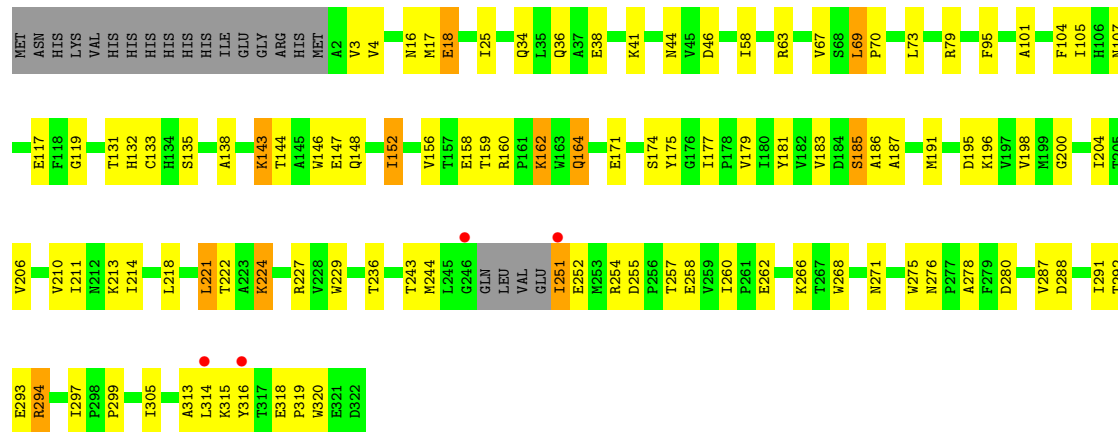




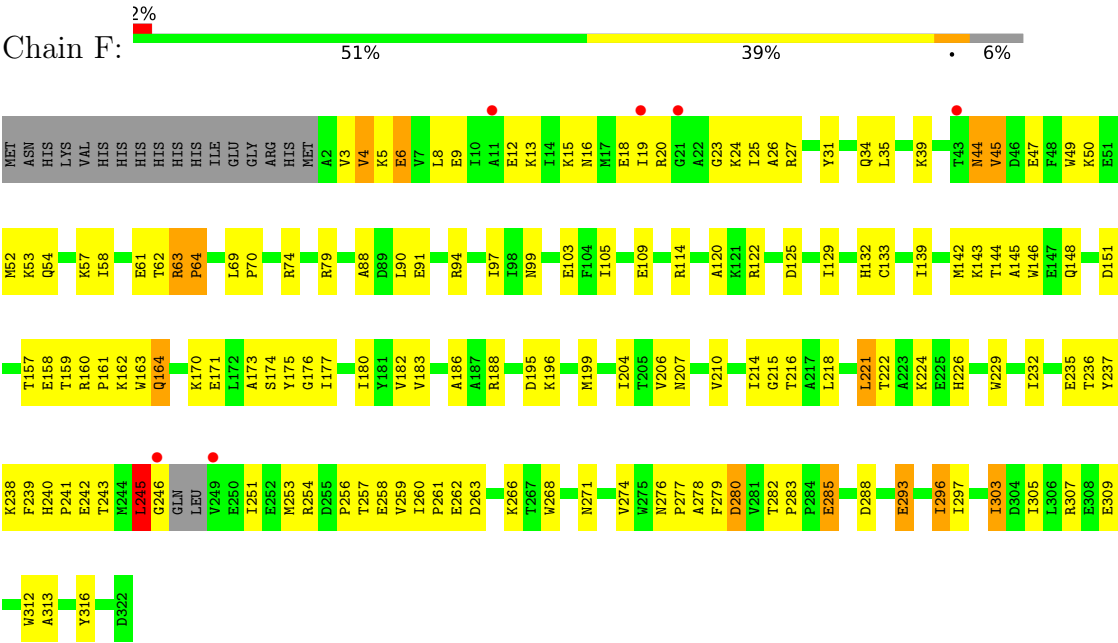
- Molecule 1: Translation initiation factor eIF-2B, delta subunit



- Molecule 1: Translation initiation factor eIF-2B, delta subunit



- Molecule 1: Translation initiation factor eIF-2B, delta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.29Å 130.81Å 132.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.66 – 2.50 43.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.66-2.50) 99.9 (43.66-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.204 , 0.266 0.204 , 0.266	Depositor DCC
R_{free} test set	3638 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15535	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: MG, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/2595	0.96	8/3514 (0.2%)
1	B	0.47	0/2610	0.96	11/3530 (0.3%)
1	C	0.40	0/2566	0.93	9/3473 (0.3%)
1	D	0.43	0/2584	0.93	6/3498 (0.2%)
1	E	0.40	0/2566	0.90	3/3473 (0.1%)
1	F	0.39	0/2582	0.90	7/3495 (0.2%)
All	All	0.42	0/15503	0.93	44/20983 (0.2%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	18	GLU	N-CA-C	-8.67	102.14	112.89
1	A	202	ASP	N-CA-C	-7.10	102.58	112.45
1	B	295	GLY	N-CA-C	6.98	120.22	111.85
1	C	162	LYS	N-CA-C	6.82	121.26	113.15
1	C	163	TRP	N-CA-C	6.79	120.86	111.90
1	E	17	MET	N-CA-C	6.78	120.90	111.74
1	C	202	ASP	N-CA-C	-6.42	103.52	112.45
1	B	72	ALA	N-CA-C	-6.19	104.61	111.36
1	F	282	THR	CA-C-N	6.18	124.17	119.66
1	F	282	THR	C-N-CA	6.18	124.17	119.66
1	C	154	VAL	N-CA-C	6.18	117.19	108.36
1	F	63	ARG	CA-C-N	6.17	127.55	119.84
1	F	63	ARG	C-N-CA	6.17	127.55	119.84
1	D	86	SER	N-CA-C	-6.10	105.41	112.92
1	D	129	ILE	N-CA-C	5.91	116.44	108.17
1	D	18	GLU	N-CA-C	-5.90	105.58	112.89
1	C	223	ALA	N-CA-C	-5.87	104.80	111.14
1	B	202	ASP	N-CA-C	-5.78	104.41	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	162	LYS	N-CA-C	5.77	119.95	113.02
1	B	210	VAL	N-CA-C	5.75	116.13	107.80
1	F	279	PHE	N-CA-C	5.69	118.84	109.85
1	F	163	TRP	N-CA-C	5.63	119.33	111.90
1	D	210	VAL	N-CA-C	5.62	115.94	107.80
1	A	14	ILE	N-CA-C	-5.59	106.75	111.56
1	A	258	GLU	N-CA-C	-5.55	105.24	112.23
1	C	298	PRO	N-CA-C	-5.48	104.72	110.58
1	A	316	TYR	N-CA-C	5.42	117.32	110.33
1	B	255	ASP	CA-C-N	5.41	125.74	119.47
1	B	255	ASP	C-N-CA	5.41	125.74	119.47
1	B	179	VAL	N-CA-C	5.41	116.26	108.48
1	A	210	VAL	N-CA-C	5.38	115.60	107.80
1	C	148	GLN	N-CA-C	-5.35	106.13	113.30
1	B	244	MET	CB-CA-C	-5.33	110.41	116.54
1	B	111	ALA	N-CA-C	5.33	116.77	111.07
1	C	297	ILE	N-CA-C	5.29	114.80	108.45
1	B	162	LYS	N-CA-C	5.16	119.33	113.19
1	C	258	GLU	N-CA-C	-5.15	105.85	111.82
1	A	179	VAL	N-CA-C	5.09	115.81	108.48
1	A	267	THR	N-CA-C	-5.09	106.47	113.30
1	B	163	TRP	N-CA-C	5.09	118.61	111.74
1	D	163	TRP	N-CA-C	5.09	118.61	111.74
1	A	148	GLN	N-CA-C	-5.08	107.10	113.15
1	F	8	LEU	N-CA-C	-5.04	106.39	112.54
1	D	309	GLU	N-CA-C	5.04	117.75	111.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2541	0	2583	114	0
1	B	2556	0	2591	110	0
1	C	2513	0	2553	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2531	0	2566	105	0
1	E	2513	0	2553	98	0
1	F	2529	0	2568	141	0
2	A	7	0	10	2	0
2	B	7	0	10	2	0
2	C	7	0	10	0	0
2	D	7	0	10	3	0
2	E	7	0	10	1	0
2	F	7	0	10	2	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
4	A	59	0	0	1	0
4	B	87	0	0	2	0
4	C	34	0	0	3	0
4	D	54	0	0	2	0
4	E	46	0	0	2	0
4	F	28	0	0	0	0
All	All	15535	0	15474	637	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 21.

All (637) 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:292:THR:HG22	1:E:294:ARG:H	1.13	1.09
1:C:164:GLN:H	1:C:164:GLN:HE21	1.06	1.02
1:B:270:LYS:HE3	1:B:270:LYS:H	1.21	0.99
1:C:218:LEU:HD22	1:D:218:LEU:HD22	1.46	0.97
1:B:292:THR:HG22	1:B:294:ARG:H	1.29	0.96
1:F:214:ILE:HD12	1:F:277:PRO:HG2	1.46	0.95
1:B:318:GLU:HG3	1:B:319:PRO:HD2	1.49	0.94
1:E:181:TYR:HB3	1:F:274:VAL:HG12	1.52	0.91
1:A:52:MET:HE2	1:A:97:ILE:HD13	1.53	0.91
1:B:270:LYS:H	1:B:270:LYS:CE	1.84	0.91
1:E:186:ALA:HB2	1:F:214:ILE:HD11	1.53	0.91
1:D:164:GLN:H	1:D:164:GLN:HE21	1.14	0.88
1:E:211:ILE:HD11	1:E:244:MET:HG3	1.53	0.88
1:C:164:GLN:H	1:C:164:GLN:NE2	1.72	0.87
1:A:164:GLN:H	1:A:164:GLN:HE21	1.17	0.87
1:E:318:GLU:HG3	1:E:319:PRO:HD2	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:GLU:O	1:D:267:THR:HG22	1.74	0.86
1:E:164:GLN:H	1:E:164:GLN:HE21	1.26	0.84
1:D:288:ASP:OD2	2:D:401:PEG:H21	1.77	0.83
1:E:187:ALA:HB3	1:F:218:LEU:HD11	1.62	0.81
1:C:52:MET:HE1	1:C:97:ILE:HG13	1.65	0.79
1:A:294:ARG:HH21	1:C:315:LYS:HD2	1.47	0.79
1:D:247:GLN:CD	1:F:122:ARG:HG3	2.08	0.79
1:B:17:MET:HE2	1:B:63:ARG:HD2	1.65	0.79
1:D:69:LEU:HB3	1:D:70:PRO:HD3	1.65	0.79
1:D:224:LYS:HA	2:D:401:PEG:H12	1.65	0.78
1:C:8:LEU:HD12	1:C:8:LEU:H	1.48	0.77
1:A:313:ALA:HB3	1:A:316:TYR:HB2	1.66	0.77
1:A:52:MET:HB3	1:A:77:MET:HE1	1.66	0.77
1:A:271:ASN:HD22	1:A:271:ASN:H	1.31	0.76
1:C:10:ILE:HD12	1:C:32:ALA:HB2	1.67	0.76
1:F:3:VAL:HG21	1:F:58:ILE:HD12	1.68	0.76
1:A:243:THR:HG22	1:A:245:LEU:H	1.48	0.76
1:B:244:MET:HB2	1:D:122:ARG:HH12	1.51	0.76
1:B:227:ARG:HE	1:E:227:ARG:HG2	1.51	0.76
1:C:164:GLN:HE21	1:C:164:GLN:N	1.84	0.76
1:F:256:PRO:HB3	1:F:274:VAL:HG23	1.68	0.76
1:F:259:VAL:HG12	1:F:260:ILE:HG13	1.68	0.75
1:A:251:ILE:HG22	1:A:252:GLU:N	2.01	0.75
1:A:33:LEU:HD11	1:A:73:LEU:HD12	1.69	0.74
1:F:132:HIS:CB	1:F:199:MET:HE3	2.17	0.74
1:D:318:GLU:HG2	1:D:320:TRP:CZ2	2.22	0.74
1:B:89:ASP:OD2	1:B:92:GLN:HG3	1.88	0.74
1:E:254:ARG:HB2	1:E:276:ASN:ND2	2.02	0.74
1:F:132:HIS:HB3	1:F:199:MET:HE3	1.68	0.74
1:D:164:GLN:H	1:D:164:GLN:NE2	1.85	0.74
1:A:164:GLN:HE21	1:A:164:GLN:N	1.86	0.74
1:B:318:GLU:HG2	1:B:320:TRP:CH2	2.23	0.73
1:A:251:ILE:HG22	1:A:252:GLU:H	1.53	0.73
1:A:5:LYS:HD3	1:A:5:LYS:N	2.03	0.73
1:A:183:VAL:HG21	1:B:160:ARG:HB3	1.69	0.73
1:F:164:GLN:H	1:F:164:GLN:HE21	1.36	0.73
1:A:224:LYS:HA	2:A:401:PEG:H41	1.70	0.73
1:B:270:LYS:HE3	1:B:270:LYS:N	2.01	0.73
1:C:297:ILE:HD13	1:C:305:ILE:HD11	1.70	0.72
1:A:139:ILE:HG22	1:A:143:LYS:HE2	1.71	0.72
1:D:52:MET:HE2	1:D:97:ILE:HG21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD13	1:B:221:LEU:HD13	1.71	0.71
1:D:297:ILE:HD13	1:D:305:ILE:HD11	1.71	0.71
1:B:318:GLU:HG2	1:B:320:TRP:CZ2	2.25	0.71
1:E:318:GLU:HG2	1:E:320:TRP:CH2	2.24	0.71
1:F:253:MET:HA	1:F:253:MET:HE2	1.72	0.71
1:C:93:LEU:O	1:C:97:ILE:HG12	1.91	0.70
1:F:260:ILE:HD13	1:F:268:TRP:CH2	2.26	0.70
1:F:288:ASP:OD2	2:F:401:PEG:H32	1.91	0.70
1:E:69:LEU:HB3	1:E:70:PRO:HD3	1.74	0.70
1:F:171:GLU:HG2	1:F:175:TYR:HE2	1.56	0.70
1:F:251:ILE:HD12	1:F:251:ILE:H	1.55	0.70
1:F:224:LYS:HA	2:F:401:PEG:H41	1.74	0.70
1:F:160:ARG:HD2	1:F:161:PRO:HA	1.74	0.70
1:E:186:ALA:CB	1:F:214:ILE:HD11	2.20	0.70
1:B:264:GLU:O	1:B:267:THR:HB	1.92	0.70
1:C:257:THR:HA	1:C:260:ILE:O	1.92	0.70
1:B:47:GLU:O	1:B:51:GLU:HG3	1.91	0.69
1:E:211:ILE:CD1	1:E:244:MET:HG3	2.22	0.69
1:F:307:ARG:HD3	1:F:312:TRP:O	1.90	0.69
1:A:143:LYS:HD3	1:A:175:TYR:CE2	2.27	0.69
1:F:164:GLN:H	1:F:164:GLN:NE2	1.89	0.69
1:E:143:LYS:HE2	1:E:147:GLU:HG3	1.73	0.69
1:A:160:ARG:HD3	1:B:158:GLU:OE2	1.93	0.69
1:F:199:MET:HE2	1:F:216:THR:HG23	1.73	0.69
1:F:199:MET:CE	1:F:216:THR:HG23	2.23	0.68
1:C:76:VAL:HG23	1:C:77:MET:N	2.08	0.68
1:C:242:GLU:HG2	1:C:243:THR:H	1.58	0.68
1:A:144:THR:O	1:A:148:GLN:HG3	1.93	0.68
1:D:182:VAL:CG1	1:D:186:ALA:HB3	2.24	0.68
1:D:247:GLN:OE1	1:F:122:ARG:HG3	1.92	0.68
1:C:221:LEU:HD13	1:D:221:LEU:HD13	1.74	0.68
4:C:603:HOH:O	1:D:183:VAL:HG13	1.93	0.68
1:C:211:ILE:HD11	1:C:244:MET:HG2	1.77	0.67
1:C:270:LYS:HE3	1:C:270:LYS:H	1.60	0.67
1:F:114:ARG:HG3	1:F:114:ARG:HH11	1.59	0.67
1:D:243:THR:HG22	1:D:247:GLN:HG2	1.75	0.67
1:E:183:VAL:HG13	4:E:617:HOH:O	1.94	0.66
1:A:210:VAL:HG21	1:A:232:ILE:HG13	1.78	0.66
1:A:305:ILE:HD11	1:C:314:LEU:HD12	1.76	0.66
1:C:144:THR:O	1:C:148:GLN:HG3	1.95	0.66
1:D:52:MET:HE2	1:D:97:ILE:HD13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:HG22	1:A:90:LEU:N	2.10	0.66
1:B:122:ARG:HE	1:F:246:GLY:HA2	1.61	0.66
1:E:255:ASP:OD2	1:E:257:THR:HB	1.96	0.66
1:C:145:ALA:O	1:C:150:LYS:HB2	1.95	0.65
1:B:132:HIS:HD2	1:B:157:THR:OG1	1.80	0.65
1:C:270:LYS:H	1:C:270:LYS:CE	2.09	0.65
1:E:160:ARG:HB3	1:F:183:VAL:HG21	1.79	0.65
1:B:17:MET:CE	1:B:63:ARG:HD2	2.25	0.65
1:B:247:GLN:HE22	1:B:252:GLU:HB2	1.60	0.65
1:B:236:THR:HG23	1:B:292:THR:HG23	1.79	0.65
1:F:13:LYS:HB3	1:F:19:ILE:HG13	1.79	0.65
1:C:13:LYS:HB3	1:C:19:ILE:HG12	1.79	0.65
1:C:195:ASP:O	1:C:196:LYS:HD2	1.97	0.64
1:B:164:GLN:H	1:B:164:GLN:HE21	1.45	0.64
1:F:235:GLU:OE1	1:F:238:LYS:HE3	1.97	0.64
1:B:89:ASP:CG	1:B:92:GLN:HE21	2.05	0.64
1:D:89:ASP:H	1:D:92:GLN:NE2	1.96	0.64
1:C:4:VAL:HG22	1:C:6:GLU:H	1.61	0.64
1:B:182:VAL:HG13	1:B:186:ALA:HB3	1.80	0.64
1:E:133:CYS:HA	1:E:159:THR:HG21	1.79	0.64
1:A:243:THR:O	1:A:244:MET:HE2	1.98	0.63
1:D:44:ASN:O	1:D:90:LEU:HD13	1.98	0.63
1:D:164:GLN:HE21	1:D:164:GLN:N	1.92	0.63
1:F:49:TRP:NE1	1:F:53:LYS:HD3	2.12	0.63
1:A:164:GLN:H	1:A:164:GLN:NE2	1.94	0.63
1:A:317:THR:HG22	1:A:318:GLU:H	1.61	0.63
1:B:196:LYS:HD3	1:B:229:TRP:HB3	1.79	0.63
1:E:236:THR:HG23	1:E:292:THR:HG23	1.80	0.63
1:F:256:PRO:HB3	1:F:274:VAL:CG2	2.28	0.63
1:B:247:GLN:NE2	1:B:252:GLU:HB2	2.13	0.63
1:C:6:GLU:HB3	1:C:35:LEU:HD13	1.81	0.63
1:D:6:GLU:HB3	1:D:35:LEU:HD13	1.80	0.63
1:E:160:ARG:CB	1:F:183:VAL:HG21	2.29	0.63
1:F:3:VAL:HG21	1:F:58:ILE:CD1	2.28	0.63
1:A:251:ILE:CG2	1:A:252:GLU:H	2.11	0.63
1:C:89:ASP:OD1	1:C:92:GLN:HB2	1.99	0.63
1:F:199:MET:HE1	1:F:216:THR:HA	1.79	0.63
1:B:317:THR:HB	1:B:321:GLU:HB2	1.79	0.62
1:A:305:ILE:CD1	1:C:314:LEU:HD12	2.30	0.62
1:F:133:CYS:HA	1:F:159:THR:HG21	1.82	0.62
1:E:44:ASN:HD21	1:E:46:ASP:HB2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PRO:HB2	1:A:74:ARG:HH12	1.65	0.62
1:E:41:LYS:HA	1:E:41:LYS:HE2	1.81	0.62
1:B:5:LYS:HG3	1:B:6:GLU:OE1	2.00	0.62
1:D:4:VAL:HG12	1:D:6:GLU:H	1.63	0.62
1:A:317:THR:HG22	1:A:318:GLU:N	2.15	0.61
1:B:34:GLN:O	1:B:38:GLU:HG3	1.99	0.61
1:D:45:VAL:HG22	1:D:90:LEU:N	2.15	0.61
1:E:214:ILE:HD12	1:E:280:ASP:HB3	1.82	0.61
1:E:318:GLU:HG2	1:E:320:TRP:CZ2	2.35	0.61
1:F:50:LYS:O	1:F:54:GLN:HG3	2.00	0.61
1:D:314:LEU:HD11	1:F:297:ILE:CG2	2.30	0.61
1:E:292:THR:HG22	1:E:294:ARG:N	1.99	0.61
1:F:254:ARG:HG3	1:F:278:ALA:HB2	1.81	0.61
1:A:240:HIS:CD2	1:A:241:PRO:HD2	2.35	0.61
1:D:314:LEU:HD11	1:F:297:ILE:HG21	1.81	0.61
1:A:70:PRO:HB2	1:A:74:ARG:NH1	2.16	0.61
1:F:44:ASN:C	1:F:44:ASN:HD22	2.08	0.61
1:E:292:THR:HG21	1:E:294:ARG:HG3	1.83	0.61
1:F:52:MET:HE2	1:F:97:ILE:HG21	1.83	0.61
1:A:264:GLU:O	1:A:267:THR:HB	2.01	0.61
1:D:144:THR:O	1:D:148:GLN:HG3	2.00	0.61
1:D:269:PRO:HD2	1:D:272:ILE:HD12	1.83	0.61
1:B:285:GLU:CD	1:B:285:GLU:H	2.08	0.61
1:D:79:ARG:HH21	1:D:79:ARG:HG3	1.66	0.61
1:F:105:ILE:O	1:F:109:GLU:HG3	2.00	0.61
1:F:188:ARG:HA	1:F:222:THR:HG21	1.83	0.61
1:A:251:ILE:HG22	1:A:252:GLU:HG2	1.83	0.60
1:B:89:ASP:H	1:B:92:GLN:NE2	1.99	0.60
4:C:604:HOH:O	1:D:182:VAL:HG13	2.02	0.60
1:E:144:THR:O	1:E:148:GLN:HG3	2.00	0.59
1:A:5:LYS:HG2	1:A:6:GLU:OE2	2.01	0.59
1:C:10:ILE:HG21	1:C:28:SER:HB3	1.84	0.59
1:C:211:ILE:CD1	1:C:244:MET:HG2	2.32	0.59
1:D:138:ALA:C	1:D:142:MET:HE3	2.28	0.59
1:A:271:ASN:HD22	1:A:271:ASN:N	1.93	0.59
1:B:314:LEU:HB3	1:D:294:ARG:HB3	1.85	0.59
1:C:76:VAL:HG23	1:C:77:MET:H	1.67	0.59
1:F:129:ILE:CD1	1:F:196:LYS:HB2	2.33	0.59
1:F:144:THR:O	1:F:148:GLN:HG3	2.03	0.59
1:B:206:VAL:HG13	1:B:241:PRO:HA	1.84	0.59
1:C:221:LEU:HD11	1:D:221:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:HD3	1:A:5:LYS:H	1.66	0.58
1:B:79:ARG:HG3	1:B:79:ARG:HH11	1.68	0.58
1:B:244:MET:HB2	1:D:122:ARG:NH1	2.18	0.58
1:E:143:LYS:O	1:E:147:GLU:HG3	2.04	0.58
1:B:227:ARG:HG2	1:E:227:ARG:CG	2.34	0.58
1:F:307:ARG:HH21	1:F:307:ARG:HG3	1.68	0.58
1:B:143:LYS:HD3	1:B:175:TYR:CE2	2.38	0.58
1:F:139:ILE:HA	1:F:142:MET:HE3	1.85	0.58
1:B:182:VAL:CG1	1:B:186:ALA:HB3	2.34	0.58
1:F:120:ALA:HB1	1:F:148:GLN:OE1	2.04	0.58
1:F:313:ALA:HB3	1:F:316:TYR:CD2	2.39	0.58
1:A:52:MET:HE2	1:A:97:ILE:HG21	1.87	0.57
1:F:251:ILE:HD12	1:F:251:ILE:N	2.19	0.57
1:C:49:TRP:NE1	1:C:53:LYS:HE3	2.19	0.57
1:E:292:THR:CG2	1:E:293:GLU:N	2.67	0.57
1:A:15:LYS:C	1:A:17:MET:H	2.12	0.57
1:E:34:GLN:O	1:E:38:GLU:HG3	2.04	0.57
1:E:206:VAL:CG1	1:E:243:THR:HG22	2.34	0.57
1:F:235:GLU:HG2	1:F:237:TYR:CZ	2.39	0.57
1:E:236:THR:HG23	1:E:292:THR:CG2	2.34	0.57
1:F:240:HIS:HD2	1:F:241:PRO:HD2	1.68	0.57
1:B:67:VAL:HG23	1:B:240:HIS:CE1	2.40	0.57
1:E:183:VAL:HG12	1:E:185:SER:H	1.69	0.57
1:A:70:PRO:O	1:A:74:ARG:HG3	2.04	0.57
1:A:294:ARG:NH2	1:C:315:LYS:HD2	2.19	0.57
1:B:164:GLN:H	1:B:164:GLN:NE2	2.01	0.57
1:E:171:GLU:O	1:E:174:SER:HB3	2.05	0.57
1:A:31:TYR:CE2	1:A:35:LEU:HD11	2.39	0.57
1:A:251:ILE:CG2	1:A:252:GLU:N	2.66	0.57
1:C:54:GLN:O	1:C:58:ILE:HG13	2.05	0.57
1:E:211:ILE:HD11	1:E:244:MET:CG	2.30	0.57
1:B:143:LYS:HD3	1:B:175:TYR:CZ	2.40	0.56
1:C:222:THR:O	1:C:226:HIS:HD2	1.87	0.56
1:D:6:GLU:HG3	1:D:39:LYS:HD2	1.86	0.56
1:E:268:TRP:CD1	1:E:268:TRP:H	2.23	0.56
1:E:292:THR:CG2	1:E:294:ARG:HG3	2.35	0.56
1:F:70:PRO:O	1:F:74:ARG:HG3	2.04	0.56
1:A:34:GLN:O	1:A:38:GLU:HG3	2.05	0.56
1:C:3:VAL:CG1	1:C:8:LEU:HD11	2.35	0.56
4:D:636:HOH:O	1:F:296:ILE:HD13	2.06	0.56
1:F:235:GLU:HA	1:F:293:GLU:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ASN:H	1:A:271:ASN:ND2	2.03	0.56
1:F:114:ARG:HG3	1:F:114:ARG:NH1	2.21	0.56
1:B:70:PRO:HB2	1:B:74:ARG:NH1	2.20	0.56
1:E:138:ALA:HB1	1:E:198:VAL:HG12	1.87	0.56
1:F:242:GLU:HG2	1:F:243:THR:N	2.20	0.55
1:F:260:ILE:HD12	1:F:274:VAL:HG11	1.88	0.55
1:C:82:ILE:HG23	1:C:83:ALA:N	2.21	0.55
1:D:40:SER:HB3	1:D:94:ARG:NH2	2.22	0.55
1:E:224:LYS:HE2	1:E:227:ARG:NH1	2.21	0.55
1:F:271:ASN:N	1:F:271:ASN:HD22	2.04	0.55
1:A:3:VAL:HG11	1:A:55:ALA:HA	1.88	0.55
1:E:195:ASP:O	1:E:196:LYS:HG3	2.06	0.55
1:A:218:LEU:HD22	1:B:218:LEU:HD22	1.89	0.55
1:D:297:ILE:HD13	1:D:305:ILE:CD1	2.37	0.55
1:C:4:VAL:HG12	1:C:36:GLN:OE1	2.07	0.55
1:D:133:CYS:HA	1:D:159:THR:HG21	1.88	0.55
1:C:270:LYS:H	1:C:270:LYS:CD	2.19	0.55
1:B:183:VAL:HG22	4:B:611:HOH:O	2.07	0.54
1:A:21:GLY:O	1:A:25:ILE:HG23	2.08	0.54
1:B:17:MET:O	1:B:20:ARG:NH2	2.40	0.54
1:D:145:ALA:O	1:D:150:LYS:HB2	2.07	0.54
1:F:222:THR:O	1:F:226:HIS:HD2	1.89	0.54
1:A:107:ASN:HD21	1:C:315:LYS:HE2	1.72	0.54
1:D:313:ALA:HB3	1:D:315:LYS:HE3	1.90	0.54
1:F:99:ASN:O	1:F:103:GLU:HG3	2.07	0.54
1:A:67:VAL:HG13	1:A:240:HIS:CD2	2.42	0.54
1:A:243:THR:HG22	1:A:244:MET:N	2.23	0.54
1:E:4:VAL:HG22	1:E:36:GLN:OE1	2.07	0.54
1:F:293:GLU:CD	1:F:293:GLU:H	2.15	0.54
1:F:20:ARG:O	1:F:24:LYS:HE3	2.08	0.54
1:D:138:ALA:O	1:D:142:MET:HE3	2.07	0.54
1:A:49:TRP:CE3	1:A:49:TRP:HA	2.43	0.54
1:B:192:LYS:NZ	1:B:192:LYS:HB3	2.23	0.54
1:F:305:ILE:O	1:F:309:GLU:HB2	2.07	0.54
1:D:42:ALA:HB2	1:D:51:GLU:OE2	2.08	0.53
1:C:221:LEU:CD1	1:D:221:LEU:HD22	2.37	0.53
1:A:3:VAL:HG11	1:A:58:ILE:HD12	1.90	0.53
1:A:17:MET:C	1:A:19:ILE:H	2.16	0.53
1:B:314:LEU:O	1:D:294:ARG:HD3	2.07	0.53
1:D:77:MET:HB3	1:D:319:PRO:HB2	1.90	0.53
1:A:158:GLU:HG3	1:A:181:TYR:OH	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:ASN:OD1	1:E:18:GLU:HG3	2.08	0.53
1:F:253:MET:HE2	1:F:277:PRO:HA	1.90	0.53
1:C:213:LYS:HD3	1:C:214:ILE:H	1.74	0.53
1:D:247:GLN:HG3	1:F:122:ARG:HE	1.74	0.53
1:C:8:LEU:HD12	1:C:8:LEU:N	2.21	0.53
1:F:6:GLU:O	1:F:9:GLU:HB3	2.08	0.53
1:B:153:LYS:HD3	1:B:180:ILE:HD11	1.90	0.53
1:C:4:VAL:CG1	1:C:7:VAL:HG23	2.39	0.53
1:E:143:LYS:NZ	1:E:175:TYR:HB3	2.23	0.53
1:E:162:LYS:HZ3	1:E:258:GLU:HB3	1.74	0.53
1:F:143:LYS:HZ3	1:F:143:LYS:HB2	1.72	0.53
1:F:146:TRP:CG	1:F:177:ILE:HG12	2.44	0.53
1:F:254:ARG:HB2	1:F:276:ASN:ND2	2.23	0.53
1:C:242:GLU:HG2	1:C:243:THR:N	2.24	0.52
1:B:133:CYS:HA	1:B:159:THR:HG21	1.90	0.52
1:C:139:ILE:HA	1:C:142:MET:HE3	1.91	0.52
1:D:143:LYS:HD2	1:D:175:TYR:CZ	2.45	0.52
1:D:318:GLU:CG	1:D:320:TRP:CZ2	2.93	0.52
1:E:158:GLU:HG3	1:E:181:TYR:OH	2.09	0.52
1:F:307:ARG:HG3	1:F:307:ARG:NH2	2.25	0.52
1:A:160:ARG:HB3	1:B:183:VAL:HG21	1.90	0.52
1:D:79:ARG:HG3	1:D:79:ARG:NH2	2.25	0.52
1:F:4:VAL:HG12	1:F:5:LYS:N	2.25	0.52
1:B:67:VAL:HG23	1:B:240:HIS:ND1	2.25	0.52
1:D:254:ARG:HB2	1:D:276:ASN:ND2	2.25	0.52
1:B:50:LYS:O	1:B:54:GLN:HG3	2.10	0.52
1:E:254:ARG:HH11	1:E:254:ARG:HG3	1.75	0.52
1:F:132:HIS:HB2	1:F:199:MET:HE3	1.89	0.52
1:A:294:ARG:HB2	1:C:314:LEU:HD13	1.92	0.52
1:C:164:GLN:NE2	1:C:164:GLN:N	2.51	0.52
1:D:227:ARG:HH11	1:D:227:ARG:HB3	1.75	0.52
1:E:196:LYS:HG2	1:E:229:TRP:HB3	1.92	0.52
1:A:54:GLN:O	1:A:58:ILE:HG13	2.10	0.52
1:D:222:THR:O	1:D:226:HIS:HD2	1.92	0.52
1:B:292:THR:HG22	1:B:293:GLU:N	2.24	0.52
1:C:161:PRO:HB3	1:C:259:VAL:HG22	1.92	0.52
1:F:236:THR:N	1:F:293:GLU:OE1	2.34	0.52
1:A:183:VAL:HG21	1:B:160:ARG:CB	2.38	0.52
1:D:105:ILE:O	1:D:109:GLU:HG3	2.09	0.52
1:A:45:VAL:HG22	1:A:90:LEU:H	1.75	0.51
1:C:79:ARG:HG3	1:C:79:ARG:HH11	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LEU:HB3	1:A:70:PRO:CD	2.41	0.51
1:A:205:THR:HG21	1:A:244:MET:HG2	1.91	0.51
1:C:287:VAL:HG13	1:C:299:PRO:HG2	1.93	0.51
1:C:235:GLU:HG3	1:C:237:TYR:CZ	2.46	0.51
1:A:6:GLU:HA	1:A:9:GLU:HG2	1.91	0.51
1:A:123:ILE:HD12	1:A:129:ILE:HD11	1.92	0.51
1:B:224:LYS:HE3	1:B:227:ARG:HH12	1.76	0.51
1:E:297:ILE:HD13	1:E:305:ILE:CD1	2.40	0.51
1:F:257:THR:HG23	1:F:261:PRO:HA	1.92	0.51
1:B:236:THR:HG23	1:B:292:THR:CG2	2.40	0.51
1:D:262:GLU:O	1:D:266:LYS:HG3	2.10	0.51
1:F:171:GLU:HG2	1:F:175:TYR:CE2	2.42	0.51
1:E:294:ARG:HE	1:E:294:ARG:C	2.19	0.51
1:F:61:GLU:HA	1:F:64:PRO:HG3	1.92	0.51
1:A:44:ASN:HB3	1:A:47:GLU:HB3	1.93	0.51
1:A:49:TRP:HA	1:A:49:TRP:HE3	1.74	0.51
1:C:8:LEU:H	1:C:8:LEU:CD1	2.20	0.51
1:E:79:ARG:HH11	1:E:79:ARG:HG3	1.76	0.51
1:D:27:ARG:HD3	1:D:108:SER:OG	2.11	0.51
1:E:67:VAL:O	1:E:70:PRO:HD2	2.11	0.51
1:B:214:ILE:HD12	1:B:280:ASP:HB3	1.94	0.50
1:C:48:PHE:O	1:C:51:GLU:HB3	2.10	0.50
1:C:319:PRO:HG2	1:C:320:TRP:CE3	2.47	0.50
1:D:84:TYR:C	1:D:86:SER:H	2.19	0.50
1:D:182:VAL:HG12	1:D:186:ALA:HB3	1.94	0.50
1:E:206:VAL:HG12	1:E:243:THR:HG22	1.92	0.50
1:F:44:ASN:ND2	1:F:47:GLU:H	2.09	0.50
1:E:186:ALA:HB2	1:F:214:ILE:CD1	2.34	0.50
1:E:213:LYS:HD3	1:E:278:ALA:O	2.10	0.50
1:E:292:THR:HG22	1:E:293:GLU:N	2.27	0.50
1:C:69:LEU:HB3	1:C:70:PRO:CD	2.42	0.50
1:F:45:VAL:HG22	1:F:90:LEU:N	2.27	0.50
1:C:49:TRP:CD1	1:C:53:LYS:HE3	2.47	0.50
1:F:45:VAL:HG11	1:F:88:ALA:O	2.12	0.50
1:A:44:ASN:HB3	1:A:47:GLU:CB	2.41	0.50
1:F:207:ASN:ND2	1:F:245:LEU:HD22	2.26	0.50
1:B:316:TYR:OH	1:D:107:ASN:ND2	2.44	0.50
1:C:69:LEU:HB3	1:C:70:PRO:HD3	1.93	0.50
1:D:20:ARG:O	1:D:24:LYS:HE2	2.12	0.50
1:C:13:LYS:CB	1:C:19:ILE:HG12	2.42	0.50
1:C:79:ARG:C	1:C:82:ILE:HG22	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:HA	1:A:9:GLU:OE2	2.12	0.49
1:A:164:GLN:N	1:A:164:GLN:NE2	2.54	0.49
1:A:181:TYR:CE2	1:B:260:ILE:HD11	2.47	0.49
1:B:314:LEU:HD11	1:D:297:ILE:CG2	2.42	0.49
1:C:4:VAL:HG13	1:C:7:VAL:HG23	1.93	0.49
1:C:76:VAL:CG2	1:C:77:MET:N	2.74	0.49
1:C:270:LYS:HD2	1:C:270:LYS:N	2.27	0.49
1:E:251:ILE:HD13	1:E:251:ILE:N	2.27	0.49
1:E:260:ILE:HG13	1:E:268:TRP:CH2	2.47	0.49
1:A:17:MET:HG2	1:A:20:ARG:HD2	1.93	0.49
1:F:63:ARG:N	1:F:64:PRO:HD3	2.27	0.49
1:F:222:THR:HG22	1:F:226:HIS:CD2	2.47	0.49
1:E:152:ILE:HD13	1:E:152:ILE:H	1.77	0.49
1:A:243:THR:HG22	1:A:244:MET:H	1.77	0.49
1:B:292:THR:CG2	1:B:293:GLU:N	2.75	0.49
1:D:45:VAL:HG11	1:D:88:ALA:O	2.13	0.49
1:B:285:GLU:HG3	4:D:604:HOH:O	2.12	0.49
1:E:251:ILE:HG12	1:E:252:GLU:N	2.27	0.49
1:F:196:LYS:HD3	1:F:229:TRP:HB3	1.94	0.49
1:A:9:GLU:O	1:A:13:LYS:HG3	2.13	0.49
1:C:10:ILE:CG2	1:C:28:SER:HB3	2.43	0.49
1:E:25:ILE:HD11	1:E:63:ARG:HH11	1.77	0.49
1:F:313:ALA:HB3	1:F:316:TYR:HD2	1.76	0.49
1:B:206:VAL:HG13	1:B:241:PRO:C	2.36	0.49
1:C:212:ASN:O	1:C:279:PHE:HB3	2.12	0.49
1:E:135:SER:OG	1:E:200:GLY:HA3	2.13	0.49
1:E:191:MET:HE3	1:E:222:THR:HG23	1.95	0.49
1:A:4:VAL:HG13	1:A:36:GLN:OE1	2.12	0.48
1:E:195:ASP:C	1:E:196:LYS:HG3	2.37	0.48
1:F:242:GLU:HG2	1:F:243:THR:H	1.77	0.48
1:A:10:ILE:O	1:A:14:ILE:HG13	2.13	0.48
1:A:15:LYS:C	1:A:17:MET:N	2.71	0.48
1:A:267:THR:HG22	1:A:268:TRP:HD1	1.78	0.48
1:C:255:ASP:O	1:C:258:GLU:HB2	2.12	0.48
1:D:182:VAL:HG11	1:D:186:ALA:HB3	1.95	0.48
1:F:69:LEU:HB3	1:F:70:PRO:CD	2.43	0.48
1:B:314:LEU:HD22	1:D:294:ARG:O	2.13	0.48
1:C:5:LYS:O	1:C:9:GLU:HB2	2.14	0.48
1:C:76:VAL:CG2	1:C:77:MET:H	2.26	0.48
1:D:40:SER:HB3	1:D:94:ARG:HH21	1.79	0.48
1:F:23:GLY:HA3	1:F:27:ARG:HH12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LYS:HE2	1:B:164:GLN:OE1	2.13	0.48
1:A:211:ILE:HD13	1:A:251:ILE:HD11	1.95	0.48
1:A:145:ALA:O	1:A:150:LYS:HB2	2.13	0.48
1:B:78:HIS:CE1	1:B:311:GLY:HA3	2.48	0.48
1:C:133:CYS:HA	1:C:159:THR:HG21	1.95	0.48
1:D:4:VAL:HG12	1:D:6:GLU:HG2	1.96	0.48
1:F:162:LYS:HE2	1:F:164:GLN:OE1	2.13	0.48
1:C:35:LEU:C	1:C:37:ALA:H	2.22	0.48
1:C:35:LEU:C	1:C:37:ALA:N	2.71	0.48
1:C:102:LYS:HD3	1:C:102:LYS:O	2.14	0.48
1:C:101:ALA:O	1:C:105:ILE:HG13	2.14	0.48
1:C:314:LEU:O	1:C:316:TYR:N	2.46	0.48
1:E:314:LEU:H	1:E:314:LEU:HD23	1.77	0.48
1:B:33:LEU:O	1:B:52:MET:HE1	2.13	0.47
1:C:269:PRO:HD2	1:C:272:ILE:HD12	1.95	0.47
1:D:4:VAL:CG1	1:D:6:GLU:HG2	2.43	0.47
1:A:159:THR:O	1:A:159:THR:HG22	2.12	0.47
1:C:307:ARG:HG2	1:C:312:TRP:O	2.13	0.47
1:D:65:THR:O	1:D:66:ALA:C	2.56	0.47
1:D:89:ASP:CG	1:D:90:LEU:N	2.72	0.47
1:E:156:VAL:HG23	1:E:179:VAL:HG13	1.96	0.47
1:B:105:ILE:O	1:B:109:GLU:HG3	2.14	0.47
1:C:3:VAL:HG13	1:C:8:LEU:HD11	1.96	0.47
1:F:253:MET:CE	1:F:277:PRO:HA	2.44	0.47
1:A:186:ALA:HA	1:B:214:ILE:HD11	1.96	0.47
1:B:291:ILE:HD13	1:B:296:ILE:HG12	1.94	0.47
1:C:270:LYS:CD	1:C:270:LYS:N	2.77	0.47
1:F:9:GLU:O	1:F:12:GLU:HB2	2.14	0.47
1:A:17:MET:C	1:A:19:ILE:N	2.73	0.47
1:D:182:VAL:HG12	1:D:183:VAL:N	2.29	0.47
1:A:257:THR:HA	1:A:260:ILE:O	2.14	0.47
1:B:79:ARG:HG3	1:B:79:ARG:NH1	2.30	0.47
1:B:278:ALA:HA	4:B:668:HOH:O	2.14	0.47
1:F:20:ARG:HA	1:F:25:ILE:HD11	1.97	0.47
1:A:45:VAL:HG11	1:A:88:ALA:O	2.15	0.47
1:B:70:PRO:HB2	1:B:74:ARG:HH12	1.80	0.47
1:A:122:ARG:CZ	1:C:243:THR:HG22	2.45	0.46
1:C:49:TRP:HA	1:C:49:TRP:CE3	2.50	0.46
1:C:65:THR:HG23	1:C:66:ALA:N	2.30	0.46
1:D:45:VAL:HG22	1:D:90:LEU:HB2	1.96	0.46
1:D:253:MET:HE1	1:D:275:TRP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:ASN:N	1:F:271:ASN:ND2	2.62	0.46
1:D:44:ASN:C	1:D:90:LEU:HD13	2.40	0.46
1:E:3:VAL:HG21	1:E:58:ILE:HD12	1.98	0.46
1:B:78:HIS:CG	1:B:311:GLY:HA3	2.50	0.46
1:B:247:GLN:HG3	1:B:247:GLN:O	2.15	0.46
4:E:619:HOH:O	1:F:182:VAL:HG23	2.15	0.46
1:B:206:VAL:CG1	1:B:241:PRO:HA	2.44	0.46
1:C:16:ASN:O	1:C:17:MET:HB2	2.16	0.46
1:A:52:MET:HE3	1:A:77:MET:HE1	1.97	0.46
1:C:318:GLU:HG3	1:C:319:PRO:HD2	1.97	0.46
1:C:241:PRO:HA	1:C:306:LEU:CD1	2.46	0.46
1:F:31:TYR:CZ	1:F:35:LEU:HD21	2.51	0.46
1:F:129:ILE:HD12	1:F:196:LYS:HB2	1.98	0.46
1:F:4:VAL:CG1	1:F:5:LYS:N	2.78	0.46
1:F:44:ASN:C	1:F:44:ASN:ND2	2.74	0.46
1:C:262:GLU:O	1:C:266:LYS:HG2	2.16	0.46
1:F:162:LYS:HB2	1:F:164:GLN:HE22	1.81	0.46
1:A:211:ILE:HG21	1:A:251:ILE:HD12	1.97	0.46
1:F:260:ILE:HD13	1:F:268:TRP:CZ3	2.51	0.46
1:B:269:PRO:C	1:B:271:ASN:N	2.74	0.45
1:C:263:ASP:OD2	1:C:264:GLU:N	2.49	0.45
1:D:42:ALA:HA	1:D:47:GLU:OE2	2.16	0.45
1:C:40:SER:HB2	1:C:51:GLU:OE2	2.16	0.45
1:D:36:GLN:O	1:D:40:SER:HB2	2.16	0.45
1:D:236:THR:N	1:D:293:GLU:OE2	2.47	0.45
1:E:254:ARG:HG3	1:E:254:ARG:NH1	2.31	0.45
1:E:318:GLU:CG	1:E:319:PRO:HD2	2.36	0.45
1:F:170:LYS:O	1:F:173:ALA:HB3	2.17	0.45
1:B:0:HIS:HE1	1:B:51:GLU:OE2	2.00	0.45
1:B:289:VAL:HB	1:B:296:ILE:HG23	1.98	0.45
1:C:8:LEU:O	1:C:12:GLU:HG3	2.16	0.45
1:D:16:ASN:O	1:D:17:MET:HB2	2.17	0.45
2:E:401:PEG:H21	2:E:401:PEG:H42	1.73	0.45
1:D:77:MET:CB	1:D:319:PRO:HB2	2.46	0.45
1:E:271:ASN:HD21	1:F:173:ALA:CA	2.30	0.45
1:A:95:PHE:O	1:A:99:ASN:HB2	2.17	0.45
1:C:7:VAL:C	1:C:9:GLU:N	2.75	0.45
1:A:25:ILE:HG13	1:A:26:ALA:N	2.27	0.45
1:A:25:ILE:HD11	1:A:69:LEU:HB2	1.99	0.45
1:C:45:VAL:HG11	1:C:88:ALA:O	2.16	0.45
1:F:57:LYS:O	1:F:61:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ALA:HB1	1:A:62:THR:HG21	1.99	0.45
1:B:89:ASP:H	1:B:92:GLN:HE21	1.63	0.45
1:C:49:TRP:HA	1:C:49:TRP:HE3	1.82	0.45
1:C:49:TRP:CZ3	1:C:52:MET:HE3	2.52	0.45
1:D:34:GLN:O	1:D:38:GLU:HG3	2.17	0.45
1:F:206:VAL:CG1	1:F:241:PRO:HA	2.46	0.45
1:B:224:LYS:HD2	2:B:401:PEG:H31	1.98	0.45
1:C:214:ILE:HD11	1:D:186:ALA:HA	1.99	0.45
1:D:317:THR:O	1:D:317:THR:HG22	2.17	0.45
1:A:107:ASN:HD21	1:C:315:LYS:CE	2.30	0.45
1:D:307:ARG:HD2	1:D:308:GLU:OE1	2.17	0.45
1:E:262:GLU:O	1:E:266:LYS:HG3	2.17	0.45
1:F:6:GLU:N	1:F:6:GLU:OE1	2.49	0.45
1:F:91:GLU:OE1	1:F:94:ARG:NH1	2.50	0.45
1:B:144:THR:O	1:B:148:GLN:HG3	2.17	0.44
1:C:26:ALA:HB2	1:C:68:SER:HB2	1.98	0.44
1:C:221:LEU:HD13	1:D:221:LEU:CD1	2.43	0.44
1:E:143:LYS:HE2	1:E:147:GLU:CG	2.46	0.44
1:F:210:VAL:HG21	1:F:232:ILE:HG13	1.99	0.44
1:B:207:ASN:OD1	1:D:298:PRO:HB3	2.16	0.44
1:F:23:GLY:O	1:F:26:ALA:HB3	2.17	0.44
1:B:70:PRO:O	1:B:74:ARG:HG3	2.18	0.44
1:B:78:HIS:CD2	1:B:311:GLY:HA3	2.53	0.44
1:C:33:LEU:HD11	1:C:73:LEU:HG	1.98	0.44
1:D:206:VAL:HG13	1:D:241:PRO:HA	1.98	0.44
1:C:195:ASP:C	1:C:196:LYS:HD2	2.43	0.44
1:D:26:ALA:HB2	1:D:68:SER:HB2	1.99	0.44
1:E:314:LEU:H	1:E:314:LEU:CD2	2.29	0.44
1:F:239:PHE:N	1:F:239:PHE:CD2	2.84	0.44
1:B:26:ALA:HB2	1:B:68:SER:HB2	2.00	0.44
1:B:153:LYS:HD3	1:B:180:ILE:CD1	2.47	0.44
1:D:1:MET:HA	1:D:54:GLN:HE21	1.82	0.44
1:E:164:GLN:HE21	1:E:164:GLN:N	2.05	0.44
1:A:59:LEU:O	1:A:69:LEU:HD21	2.18	0.44
1:E:177:ILE:O	1:E:179:VAL:HG23	2.18	0.44
1:E:181:TYR:CE2	1:F:260:ILE:HD11	2.52	0.44
1:F:15:LYS:HB2	1:F:62:THR:HB	1.99	0.44
1:D:45:VAL:HG12	1:D:45:VAL:O	2.18	0.44
1:E:95:PHE:CD1	1:E:95:PHE:C	2.96	0.44
1:F:182:VAL:HG22	1:F:186:ALA:HB3	1.98	0.44
1:F:174:SER:C	1:F:176:GLY:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:PRO:HA	1:C:306:LEU:HD13	2.00	0.44
1:E:159:THR:O	1:E:159:THR:HG22	2.18	0.44
1:E:204:ILE:HD12	1:E:210:VAL:HG22	2.00	0.44
1:F:297:ILE:HD13	1:F:305:ILE:CD1	2.48	0.44
1:A:133:CYS:HA	1:A:159:THR:HG21	2.00	0.43
1:C:114:ARG:O	1:C:117:GLU:HB3	2.18	0.43
1:D:288:ASP:CG	2:D:401:PEG:H21	2.41	0.43
1:B:50:LYS:HE3	1:B:50:LYS:HB2	1.86	0.43
1:C:135:SER:O	1:C:139:ILE:HG13	2.18	0.43
1:E:160:ARG:HB2	1:F:183:VAL:HG21	2.01	0.43
1:F:125:ASP:OD1	1:F:151:ASP:N	2.48	0.43
1:E:268:TRP:H	1:E:268:TRP:HD1	1.64	0.43
1:B:52:MET:HG2	1:B:97:ILE:CD1	2.48	0.43
1:B:88:ALA:HB1	1:B:92:GLN:HB2	2.00	0.43
1:C:158:GLU:HG3	1:C:181:TYR:OH	2.17	0.43
1:C:160:ARG:HB3	1:C:161:PRO:HA	2.00	0.43
1:E:221:LEU:HD13	1:F:221:LEU:HD13	2.01	0.43
1:E:297:ILE:HD13	1:E:305:ILE:HD11	2.00	0.43
1:A:6:GLU:HA	1:A:9:GLU:CG	2.48	0.43
1:A:16:ASN:HB2	1:A:18:GLU:HG3	2.00	0.43
1:C:69:LEU:HD13	1:C:69:LEU:C	2.43	0.43
1:A:224:LYS:HG3	1:A:286:TYR:CD1	2.54	0.43
1:C:153:LYS:HE2	1:C:180:ILE:HD11	1.99	0.43
1:E:313:ALA:HB3	1:E:315:LYS:HG2	2.00	0.43
1:F:52:MET:CE	1:F:97:ILE:HG21	2.49	0.43
1:F:263:ASP:HA	1:F:266:LYS:CD	2.48	0.43
1:F:283:PRO:HB3	1:F:285:GLU:OE2	2.19	0.43
1:B:307:ARG:HG3	1:B:307:ARG:HH11	1.83	0.43
1:C:40:SER:H	1:C:94:ARG:NH2	2.16	0.43
1:E:131:THR:OG1	1:E:132:HIS:N	2.52	0.43
1:B:292:THR:HG23	1:B:293:GLU:OE1	2.19	0.43
1:E:119:GLY:CA	1:E:291:ILE:HD13	2.48	0.43
1:F:16:ASN:C	1:F:18:GLU:H	2.26	0.43
1:A:288:ASP:OD1	2:A:401:PEG:H31	2.19	0.43
1:B:153:LYS:HA	1:B:178:PRO:HG2	1.99	0.43
1:D:46:ASP:O	1:D:50:LYS:HB2	2.18	0.43
1:F:204:ILE:HD12	1:F:210:VAL:HG22	2.01	0.43
1:A:69:LEU:O	1:A:73:LEU:HD22	2.19	0.43
1:B:134:HIS:HE1	1:B:171:GLU:OE1	2.02	0.43
1:C:319:PRO:HG2	1:C:320:TRP:HE3	1.84	0.43
1:A:4:VAL:HG22	1:A:7:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:LEU:HD23	1:C:314:LEU:HA	1.82	0.42
1:D:318:GLU:HG3	1:D:320:TRP:CH2	2.54	0.42
1:E:146:TRP:HB2	1:E:152:ILE:HD11	2.01	0.42
1:A:48:PHE:HB2	1:A:90:LEU:CD1	2.49	0.42
1:C:318:GLU:HG2	1:C:320:TRP:CZ2	2.53	0.42
1:D:4:VAL:HG12	1:D:5:LYS:N	2.33	0.42
1:A:52:MET:CE	1:A:97:ILE:HG21	2.49	0.42
1:A:160:ARG:CB	1:B:183:VAL:HG21	2.49	0.42
1:A:314:LEU:C	1:A:314:LEU:HD13	2.45	0.42
1:E:275:TRP:CH2	1:F:180:ILE:HD13	2.55	0.42
1:A:78:HIS:CG	1:A:311:GLY:HA3	2.54	0.42
1:C:4:VAL:CG2	1:C:6:GLU:HG2	2.50	0.42
1:D:52:MET:CE	1:D:97:ILE:HG21	2.45	0.42
1:E:268:TRP:CD1	1:E:268:TRP:N	2.88	0.42
1:F:143:LYS:HD3	1:F:175:TYR:CE1	2.54	0.42
1:F:143:LYS:NZ	1:F:175:TYR:CZ	2.87	0.42
1:C:268:TRP:HA	1:C:269:PRO:HD3	1.88	0.42
1:C:313:ALA:O	1:C:316:TYR:HB2	2.18	0.42
1:D:245:LEU:HA	1:D:281:VAL:HG11	2.02	0.42
1:F:195:ASP:C	1:F:196:LYS:HG2	2.44	0.42
1:F:215:GLY:H	1:F:280:ASP:CG	2.27	0.42
1:A:49:TRP:NE1	1:A:53:LYS:HE3	2.34	0.42
1:C:211:ILE:HD11	1:C:244:MET:CG	2.48	0.42
1:C:270:LYS:H	1:C:270:LYS:HD2	1.85	0.42
1:E:152:ILE:HD13	1:E:152:ILE:N	2.34	0.42
1:A:36:GLN:O	1:A:40:SER:HB2	2.20	0.42
1:B:257:THR:HA	1:B:260:ILE:O	2.20	0.42
1:D:182:VAL:CG1	1:D:183:VAL:N	2.83	0.42
1:E:313:ALA:C	1:E:315:LYS:H	2.28	0.42
1:B:222:THR:O	1:B:226:HIS:HD2	2.01	0.42
1:E:69:LEU:HB3	1:E:70:PRO:CD	2.46	0.42
1:F:303:ILE:O	1:F:307:ARG:HG2	2.19	0.42
1:A:17:MET:HE2	1:A:63:ARG:CZ	2.49	0.42
1:A:52:MET:HG3	1:A:97:ILE:CD1	2.50	0.42
1:D:11:ALA:HB1	1:D:62:THR:CG2	2.50	0.42
1:D:164:GLN:NE2	1:D:164:GLN:N	2.61	0.42
1:F:132:HIS:HA	1:F:157:THR:OG1	2.19	0.42
1:F:162:LYS:HD3	1:F:258:GLU:OE2	2.20	0.42
1:B:206:VAL:HG22	1:B:242:GLU:O	2.19	0.41
1:D:206:VAL:HG13	1:D:241:PRO:C	2.44	0.41
1:D:293:GLU:H	1:D:293:GLU:CD	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:ILE:HD13	1:F:196:LYS:HB2	2.02	0.41
1:A:49:TRP:CZ2	1:A:81:LYS:HA	2.56	0.41
1:A:283:PRO:HD2	1:A:286:TYR:CD2	2.55	0.41
1:C:199:MET:CE	1:C:216:THR:HG23	2.51	0.41
1:E:146:TRP:HE3	1:E:152:ILE:HD13	1.84	0.41
1:E:288:ASP:O	1:E:299:PRO:HD3	2.20	0.41
1:A:222:THR:O	1:A:226:HIS:HD2	2.04	0.41
1:B:8:LEU:O	1:B:12:GLU:HG2	2.20	0.41
1:B:314:LEU:HB3	1:D:294:ARG:CB	2.48	0.41
1:D:67:VAL:O	1:D:70:PRO:HD2	2.20	0.41
1:D:318:GLU:HA	1:D:319:PRO:HD3	1.96	0.41
1:B:198:VAL:HG22	1:B:231:MET:HE3	2.02	0.41
1:D:89:ASP:CG	1:D:90:LEU:H	2.29	0.41
1:A:49:TRP:CE2	1:A:53:LYS:HE3	2.56	0.41
1:B:224:LYS:HA	2:B:401:PEG:H31	2.02	0.41
1:C:33:LEU:HD13	1:C:76:VAL:HG21	2.02	0.41
1:D:313:ALA:C	1:D:315:LYS:H	2.28	0.41
1:F:239:PHE:N	1:F:239:PHE:HD2	2.18	0.41
1:F:31:TYR:CE2	1:F:35:LEU:HD11	2.56	0.41
1:A:16:ASN:CB	1:A:18:GLU:HG3	2.50	0.41
1:A:183:VAL:HG22	4:A:603:HOH:O	2.21	0.41
1:B:4:VAL:HG12	1:B:6:GLU:HG2	2.03	0.41
1:B:227:ARG:HG2	1:E:227:ARG:HG2	2.02	0.41
1:B:293:GLU:CD	1:B:293:GLU:H	2.28	0.41
1:C:90:LEU:O	1:C:94:ARG:HB2	2.21	0.41
1:C:210:VAL:HG21	1:C:232:ILE:HG13	2.03	0.41
1:F:31:TYR:O	1:F:34:GLN:N	2.54	0.41
1:F:157:THR:O	1:F:158:GLU:C	2.64	0.41
1:F:206:VAL:HG22	1:F:242:GLU:O	2.21	0.41
1:B:106:HIS:O	1:B:110:LYS:HG2	2.20	0.40
1:F:143:LYS:NZ	1:F:175:TYR:CE2	2.83	0.40
1:F:145:ALA:O	1:F:148:GLN:HB2	2.20	0.40
1:F:235:GLU:HG2	1:F:237:TYR:OH	2.21	0.40
1:B:227:ARG:HE	1:E:227:ARG:CG	2.28	0.40
1:C:293:GLU:H	1:C:293:GLU:CD	2.30	0.40
1:B:291:ILE:CD1	1:B:296:ILE:HG12	2.52	0.40
1:C:65:THR:HG23	1:C:66:ALA:H	1.85	0.40
1:C:49:TRP:C	1:C:51:GLU:N	2.79	0.40
1:D:160:ARG:HD2	1:D:161:PRO:HA	2.02	0.40
1:B:90:LEU:HD13	1:B:90:LEU:C	2.47	0.40
1:B:138:ALA:C	1:B:142:MET:HE3	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ALA:HB2	4:C:625:HOH:O	2.20	0.40
1:C:90:LEU:HD21	1:C:94:ARG:HH11	1.87	0.40
1:D:139:ILE:HA	1:D:142:MET:HE3	2.04	0.40
1:E:101:ALA:O	1:E:105:ILE:HG13	2.22	0.40
1:E:104:PHE:CD1	1:E:104:PHE:C	2.99	0.40
1:F:45:VAL:HG13	1:F:90:LEU:HA	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	318/338 (94%)	302 (95%)	14 (4%)	2 (1%)	21	38
1	B	318/338 (94%)	307 (96%)	11 (4%)	0	100	100
1	C	313/338 (93%)	287 (92%)	24 (8%)	2 (1%)	21	38
1	D	316/338 (94%)	296 (94%)	18 (6%)	2 (1%)	21	38
1	E	313/338 (93%)	301 (96%)	12 (4%)	0	100	100
1	F	315/338 (93%)	289 (92%)	23 (7%)	3 (1%)	12	24
All	All	1893/2028 (93%)	1782 (94%)	102 (5%)	9 (0%)	24	43

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	F	245	LEU
1	A	252	GLU
1	D	42	ALA
1	C	314	LEU
1	C	315	LYS

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Mol	Chain	Res	Type
1	F	4	VAL
1	F	64	PRO
1	D	269	PRO

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	268/284 (94%)	252 (94%)	16 (6%)	17	36
1	B	268/284 (94%)	251 (94%)	17 (6%)	16	34
1	C	264/284 (93%)	253 (96%)	11 (4%)	26	52
1	D	265/284 (93%)	250 (94%)	15 (6%)	18	39
1	E	264/284 (93%)	249 (94%)	15 (6%)	18	39
1	F	266/284 (94%)	252 (95%)	14 (5%)	20	42
All	All	1595/1704 (94%)	1507 (94%)	88 (6%)	19	40

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	20	ARG
1	A	25	ILE
1	A	49	TRP
1	A	73	LEU
1	A	107	ASN
1	A	151	ASP
1	A	164	GLN
1	A	221	LEU
1	A	240	HIS
1	A	242	GLU
1	A	263	ASP
1	A	267	THR
1	A	270	LYS
1	A	271	ASN

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Mol	Chain	Res	Type
1	A	314	LEU
1	B	6	GLU
1	B	17	MET
1	B	81	LYS
1	B	90	LEU
1	B	117	GLU
1	B	164	GLN
1	B	182	VAL
1	B	192	LYS
1	B	206	VAL
1	B	221	LEU
1	B	240	HIS
1	B	267	THR
1	B	270	LYS
1	B	271	ASN
1	B	285	GLU
1	B	293	GLU
1	B	308	GLU
1	C	49	TRP
1	C	73	LEU
1	C	91	GLU
1	C	102	LYS
1	C	164	GLN
1	C	221	LEU
1	C	240	HIS
1	C	243	THR
1	C	270	LYS
1	C	287	VAL
1	C	314	LEU
1	D	50	LYS
1	D	67	VAL
1	D	117	GLU
1	D	164	GLN
1	D	183	VAL
1	D	206	VAL
1	D	214	ILE
1	D	221	LEU
1	D	240	HIS
1	D	242	GLU
1	D	254	ARG
1	D	293	GLU
1	D	308	GLU

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Mol	Chain	Res	Type
1	D	317	THR
1	D	318	GLU
1	E	69	LEU
1	E	73	LEU
1	E	107	ASN
1	E	117	GLU
1	E	143	LYS
1	E	152	ILE
1	E	164	GLN
1	E	185	SER
1	E	218	LEU
1	E	221	LEU
1	E	224	LYS
1	E	251	ILE
1	E	287	VAL
1	E	294	ARG
1	E	316	TYR
1	F	6	GLU
1	F	39	LYS
1	F	44	ASN
1	F	45	VAL
1	F	79	ARG
1	F	164	GLN
1	F	221	LEU
1	F	245	LEU
1	F	262	GLU
1	F	280	ASP
1	F	285	GLU
1	F	293	GLU
1	F	296	ILE
1	F	303	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	107	ASN
1	A	134	HIS
1	A	148	GLN
1	A	164	GLN
1	A	212	ASN
1	A	226	HIS

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Mol	Chain	Res	Type
1	A	240	HIS
1	A	271	ASN
1	B	0	HIS
1	B	34	GLN
1	B	92	GLN
1	B	106	HIS
1	B	132	HIS
1	B	134	HIS
1	B	164	GLN
1	B	226	HIS
1	B	240	HIS
1	B	247	GLN
1	B	271	ASN
1	C	16	ASN
1	C	92	GLN
1	C	106	HIS
1	C	107	ASN
1	C	164	GLN
1	C	226	HIS
1	D	34	GLN
1	D	78	HIS
1	D	92	GLN
1	D	99	ASN
1	D	107	ASN
1	D	134	HIS
1	D	164	GLN
1	D	189	HIS
1	D	226	HIS
1	D	247	GLN
1	E	44	ASN
1	E	148	GLN
1	E	164	GLN
1	F	34	GLN
1	F	44	ASN
1	F	54	GLN
1	F	107	ASN
1	F	164	GLN
1	F	189	HIS
1	F	207	ASN
1	F	226	HIS
1	F	240	HIS
1	F	271	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEG	D	401	-	6,6,6	0.54	0	5,5,5	0.36	0
2	PEG	E	401	-	6,6,6	0.54	0	5,5,5	0.49	0
2	PEG	C	401	-	6,6,6	0.54	0	5,5,5	0.43	0
2	PEG	B	401	-	6,6,6	0.54	0	5,5,5	0.40	0
2	PEG	A	401	-	6,6,6	0.53	0	5,5,5	0.41	0
2	PEG	F	401	-	6,6,6	0.53	0	5,5,5	0.45	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	401	-	-	1/4/4/4	-
2	PEG	E	401	-	-	1/4/4/4	-
2	PEG	C	401	-	-	0/4/4/4	-
2	PEG	B	401	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	401	-	-	0/4/4/4	-
2	PEG	F	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	401	PEG	C4-C3-O2-C2
2	D	401	PEG	C4-C3-O2-C2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	PEG	3	0
2	E	401	PEG	1	0
2	B	401	PEG	2	0
2	A	401	PEG	2	0
2	F	401	PEG	2	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	320/338 (94%)	-0.02	13 (4%) 41 37	14, 36, 87, 104	0
1	B	322/338 (95%)	-0.40	4 (1%) 76 73	12, 29, 56, 82	0
1	C	317/338 (93%)	0.45	28 (8%) 15 14	20, 51, 109, 122	0
1	D	320/338 (94%)	0.02	14 (4%) 39 34	16, 37, 78, 115	0
1	E	317/338 (93%)	0.05	4 (1%) 75 71	24, 42, 68, 92	0
1	F	319/338 (94%)	0.35	6 (1%) 66 62	25, 48, 79, 111	0
All	All	1915/2028 (94%)	0.07	69 (3%) 46 41	12, 41, 86, 122	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	249	VAL	5.2
1	C	245	LEU	4.9
1	D	245	LEU	4.5
1	E	316	TYR	4.3
1	F	249	VAL	4.2
1	D	246	GLY	3.9
1	A	249	VAL	3.8
1	E	251	ILE	3.5
1	C	93	LEU	3.4
1	C	251	ILE	3.4
1	E	314	LEU	3.4
1	C	246	GLY	3.4
1	C	96	VAL	3.4
1	D	1	MET	3.3
1	C	2	ALA	3.3
1	A	19	ILE	3.3
1	C	3	VAL	3.2
1	E	246	GLY	3.1
1	F	43	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	314	LEU	3.0
1	D	248	LEU	3.0
1	D	2	ALA	2.9
1	B	245	LEU	2.8
1	C	65	THR	2.8
1	C	90	LEU	2.8
1	A	314	LEU	2.7
1	C	33	LEU	2.7
1	B	244	MET	2.7
1	A	248	LEU	2.6
1	C	49	TRP	2.6
1	C	43	THR	2.6
1	F	19	ILE	2.6
1	C	240	HIS	2.5
1	F	21	GLY	2.4
1	C	48	PHE	2.4
1	C	66	ALA	2.4
1	B	247	GLN	2.4
1	C	17	MET	2.4
1	D	270	LYS	2.4
1	F	246	GLY	2.4
1	C	42	ALA	2.4
1	D	87	GLY	2.4
1	A	251	ILE	2.4
1	A	17	MET	2.4
1	C	88	ALA	2.4
1	A	14	ILE	2.3
1	C	95	PHE	2.3
1	A	317	THR	2.3
1	D	316	TYR	2.3
1	C	50	LYS	2.3
1	D	65	THR	2.3
1	A	7	VAL	2.3
1	D	66	ALA	2.2
1	C	97	ILE	2.2
1	D	67	VAL	2.2
1	C	175	TYR	2.2
1	A	45	VAL	2.2
1	A	246	GLY	2.2
1	A	88	ALA	2.2
1	C	100	ALA	2.1
1	C	7	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	247	GLN	2.1
1	F	11	ALA	2.1
1	C	44	ASN	2.1
1	C	4	VAL	2.0
1	A	8	LEU	2.0
1	C	8	LEU	2.0
1	D	244	MET	2.0
1	B	-2	GLY	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	401	7/7	0.77	0.19	49,59,63,67	0
2	PEG	E	401	7/7	0.77	0.17	51,53,55,55	0
2	PEG	D	401	7/7	0.78	0.19	48,49,62,62	0
2	PEG	F	401	7/7	0.78	0.16	45,53,64,64	0
2	PEG	B	401	7/7	0.82	0.17	56,58,60,62	0
2	PEG	A	401	7/7	0.83	0.19	40,51,58,59	0
3	MG	B	411	1/1	0.87	0.24	51,51,51,51	0
3	MG	E	411	1/1	0.87	0.29	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.