



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:11 PM UTC

PDB ID : 2HLN / pdb_00002hln
Title : L-asparaginase from Erwinia carotovora in complex with glutamic acid
Authors : Kravchenko, O.V.; Kislitsin, Y.A.; Popov, A.N.; Nikonov, S.V.; Kuranova, I.P.
Deposited on : 2006-07-08
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

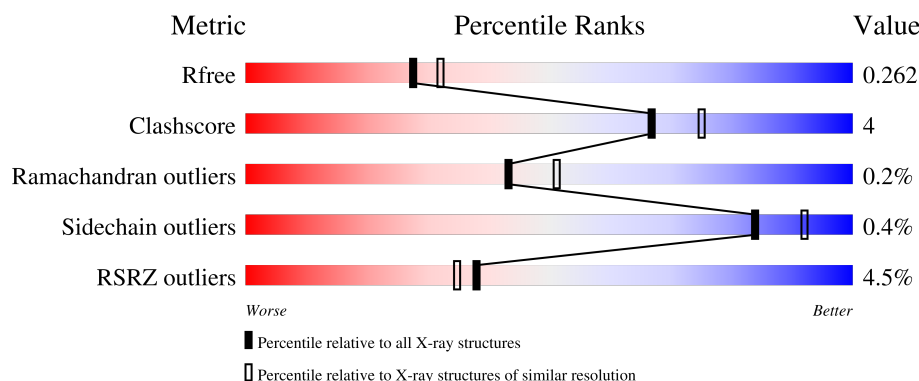
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	327	2% 84% 9% 6%
1	B	327	2% 86% 8% 6%
1	C	327	2% 88% 6% 6%
1	D	327	4% 83% 11% 6%
1	E	327	6% 83% 10% 6%

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Mol	Chain	Length	Quality of chain
1	F	327	
1	G	327	
1	H	327	
1	I	327	
1	J	327	
1	K	327	
1	L	327	

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
3	PEG	A	2002	-	-	X	-
3	PEG	K	2001	-	-	X	-

2 Entry composition

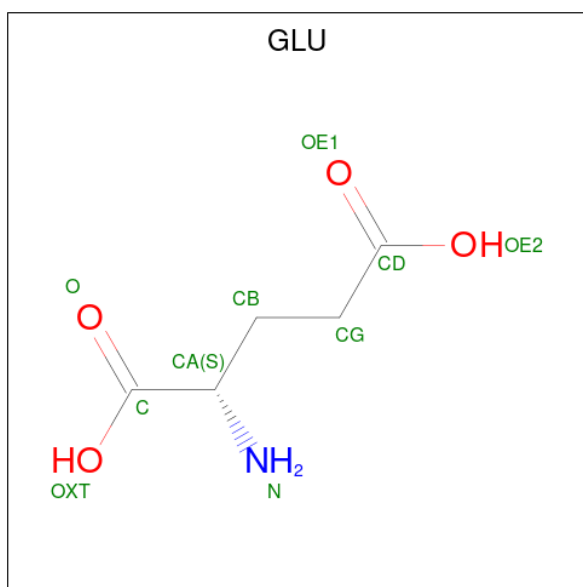
There are 4 unique types of molecules in this entry. The entry contains 29749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	1	0
			2307	1456	395	450	6			
1	B	308	Total	C	N	O	S	0	1	0
			2310	1458	398	448	6			
1	E	308	Total	C	N	O	S	0	2	0
			2313	1461	396	450	6			
1	F	308	Total	C	N	O	S	0	1	0
			2307	1456	395	450	6			
1	C	308	Total	C	N	O	S	0	2	0
			2313	1461	396	450	6			
1	D	308	Total	C	N	O	S	0	0	0
			2302	1453	395	448	6			
1	G	308	Total	C	N	O	S	0	1	0
			2307	1456	395	450	6			
1	H	308	Total	C	N	O	S	0	2	0
			2315	1461	398	450	6			
1	I	308	Total	C	N	O	S	0	0	0
			2302	1453	395	448	6			
1	J	308	Total	C	N	O	S	0	0	0
			2302	1453	395	448	6			
1	K	308	Total	C	N	O	S	0	1	0
			2310	1458	398	448	6			
1	L	308	Total	C	N	O	S	0	1	0
			2307	1456	395	450	6			

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	G	1	Total	C	N	O	0	0
			10	5	1	4		
2	H	1	Total	C	N	O	0	0
			10	5	1	4		
2	I	1	Total	C	N	O	0	0
			10	5	1	4		
2	J	1	Total	C	N	O	0	0
			10	5	1	4		
2	K	1	Total	C	N	O	0	0
			10	5	1	4		
2	L	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	G	1	Total C O 7 4 3	0	0
3	K	1	Total C O 7 4 3	0	0
3	K	1	Total C O 7 4 3	0	0
3	K	1	Total C O 7 4 3	0	0
3	K	1	Total C O 7 4 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	242	Total O 242 242	0	0
4	B	191	Total O 191 191	0	0
4	E	146	Total O 146 146	0	0
4	F	241	Total O 241 241	0	0

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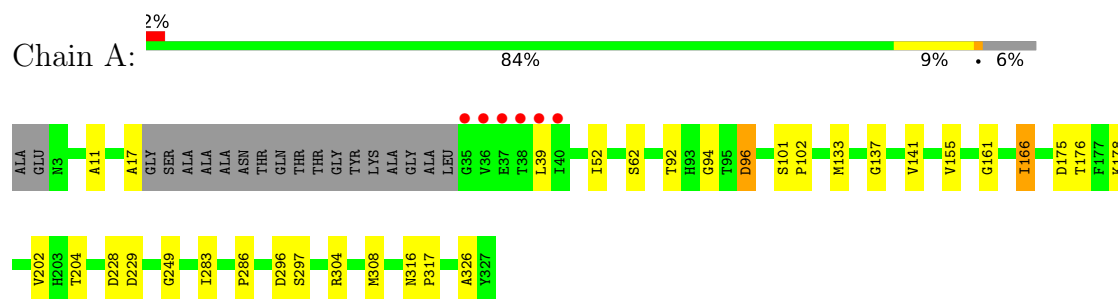
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	229	Total 229	O 229	0	0
4	D	109	Total 109	O 109	0	0
4	G	145	Total 145	O 145	0	0
4	H	129	Total 129	O 129	0	0
4	I	97	Total 97	O 97	0	0
4	J	110	Total 110	O 110	0	0
4	K	148	Total 148	O 148	0	0
4	L	91	Total 91	O 91	0	0

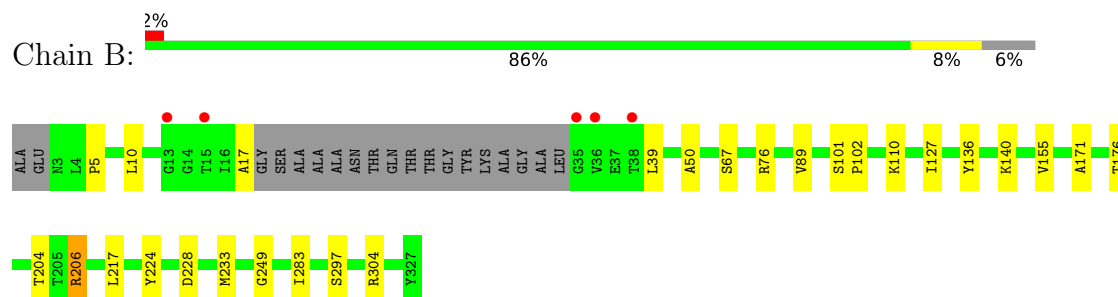
3 Residue-property plots [i](#)

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.

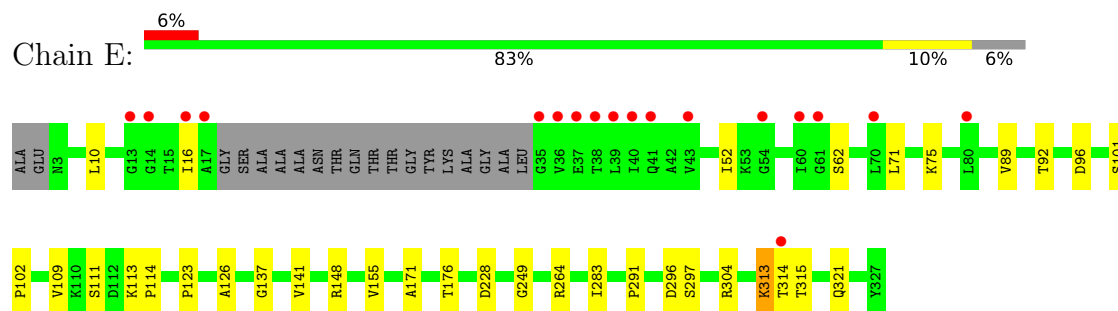
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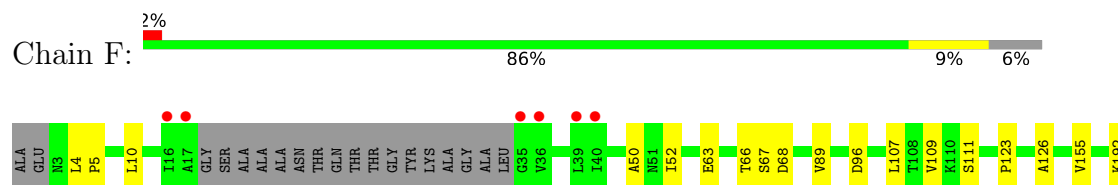
- Molecule 1: L-asparaginase



- Molecule 1: L-asparaginase

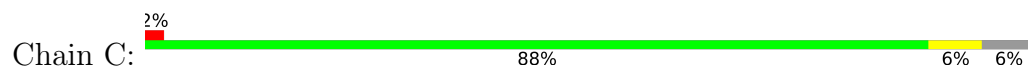


- Molecule 1: L-asparaginase

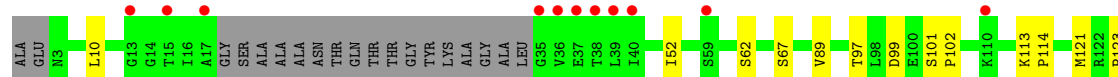
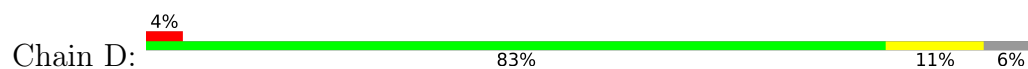




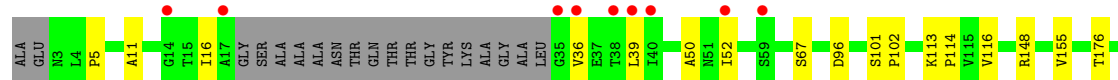
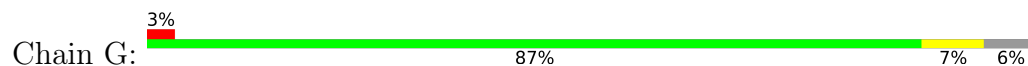
- Molecule 1: L-asparaginase



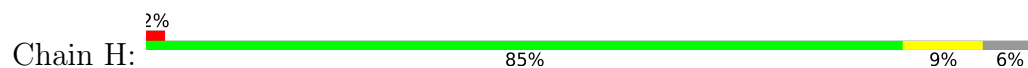
- Molecule 1: L-asparaginase



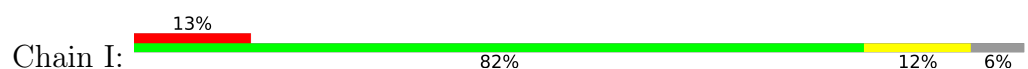
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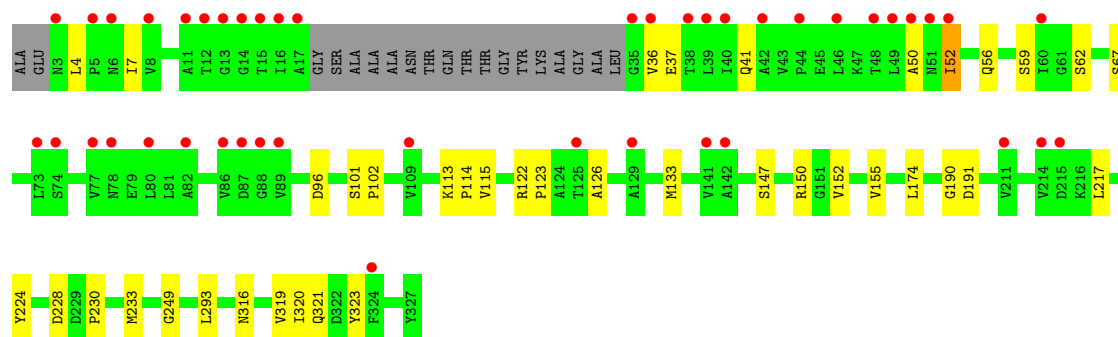


- Molecule 1: L-asparaginase

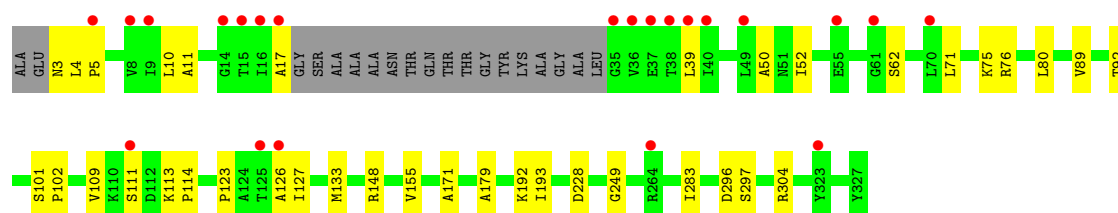
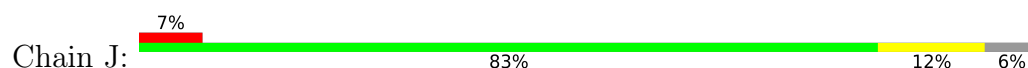


- Molecule 1: L-asparaginase

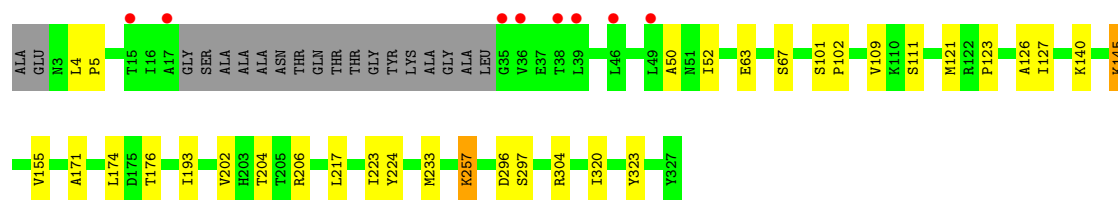
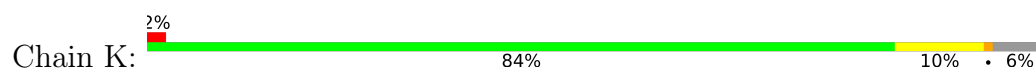




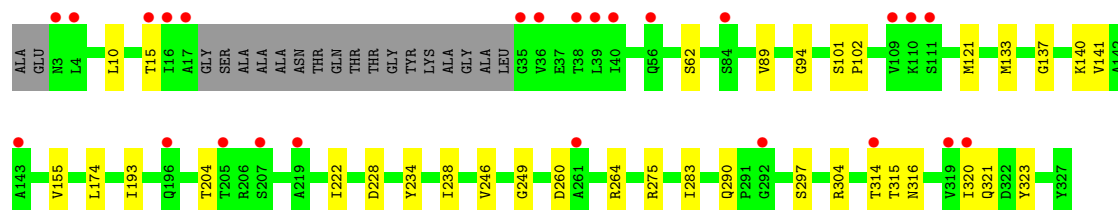
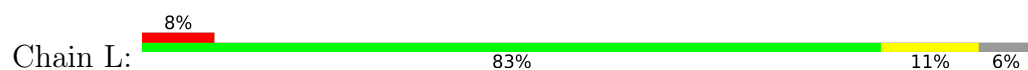
• Molecule 1: L-asparaginase



• Molecule 1: L-asparaginase



• Molecule 1: L-asparaginase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.11Å 123.67Å 197.45Å 90.00° 90.92° 90.00°	Depositor
Resolution (Å)	19.98 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.1 (19.98-2.20) 90.9 (19.98-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.267 0.217 , 0.262	Depositor DCC
R_{free} test set	9022 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29749	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.40	0/2344	0.86	8/3181 (0.3%)
1	B	0.40	0/2347	0.83	4/3184 (0.1%)
1	C	0.41	0/2353	0.82	3/3192 (0.1%)
1	D	0.39	0/2336	0.83	5/3170 (0.2%)
1	E	0.39	0/2353	0.83	7/3192 (0.2%)
1	F	0.41	0/2344	0.83	4/3181 (0.1%)
1	G	0.39	0/2344	0.83	6/3181 (0.2%)
1	H	0.38	0/2355	0.85	6/3195 (0.2%)
1	I	0.39	0/2336	0.83	6/3170 (0.2%)
1	J	0.40	0/2336	0.83	6/3170 (0.2%)
1	K	0.40	0/2347	0.82	4/3184 (0.1%)
1	L	0.39	0/2344	0.81	2/3181 (0.1%)
All	All	0.40	0/28139	0.83	61/38181 (0.2%)

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	GLY	N-CA-C	7.05	120.08	112.33
1	D	52	ILE	N-CA-C	6.58	117.34	107.80
1	I	52	ILE	N-CA-C	6.54	117.33	108.17
1	E	249	GLY	N-CA-C	6.47	120.82	112.54
1	F	52	ILE	N-CA-C	6.34	117.05	108.17
1	A	176	THR	N-CA-C	6.26	118.10	111.28
1	H	52	ILE	N-CA-C	6.10	117.27	108.48
1	F	155	VAL	N-CA-C	6.05	116.91	107.28
1	C	249	GLY	N-CA-C	6.02	120.25	112.54
1	J	155	VAL	N-CA-C	6.00	116.25	107.37
1	K	155	VAL	N-CA-C	5.95	116.74	107.28
1	E	155	VAL	N-CA-C	5.93	116.72	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	249	GLY	N-CA-C	5.93	120.14	112.54
1	G	52	ILE	N-CA-C	5.93	116.40	107.80
1	C	155	VAL	N-CA-C	5.84	116.56	107.28
1	A	229	ASP	CA-C-N	5.83	125.76	119.76
1	A	229	ASP	C-N-CA	5.83	125.76	119.76
1	B	155	VAL	N-CA-C	5.81	116.52	107.28
1	G	155	VAL	N-CA-C	5.80	116.50	107.28
1	L	249	GLY	N-CA-C	5.74	119.89	112.54
1	A	52	ILE	N-CA-C	5.73	116.84	108.53
1	H	155	VAL	N-CA-C	5.73	116.39	107.28
1	D	155	VAL	N-CA-C	5.70	116.34	107.28
1	A	155	VAL	N-CA-C	5.66	116.01	107.75
1	I	155	VAL	N-CA-C	5.64	115.72	107.37
1	I	249	GLY	N-CA-C	5.62	119.73	112.54
1	I	316	ASN	CA-C-N	5.53	124.72	118.97
1	I	316	ASN	C-N-CA	5.53	124.72	118.97
1	G	96	ASP	N-CA-C	5.49	117.27	111.28
1	H	171	ALA	N-CA-C	5.46	117.23	111.28
1	E	96	ASP	N-CA-C	5.44	117.21	111.28
1	G	249	GLY	N-CA-C	5.42	121.58	112.85
1	H	229	ASP	CA-C-N	5.41	125.17	119.76
1	H	229	ASP	C-N-CA	5.41	125.17	119.76
1	G	176	THR	N-CA-C	5.41	117.87	111.33
1	L	155	VAL	N-CA-C	5.38	115.84	107.28
1	J	52	ILE	N-CA-C	5.27	115.90	108.36
1	J	171	ALA	N-CA-C	5.27	117.02	111.28
1	A	166	ILE	N-CA-C	5.26	115.88	109.30
1	B	249	GLY	N-CA-C	5.26	120.56	112.51
1	J	249	GLY	N-CA-C	5.25	120.55	112.51
1	E	176	THR	N-CA-C	5.25	117.68	111.33
1	F	96	ASP	N-CA-C	5.24	116.99	111.28
1	K	171	ALA	N-CA-C	5.23	117.72	111.71
1	E	52	ILE	N-CA-C	5.22	115.82	108.36
1	F	249	GLY	N-CA-C	5.19	120.45	112.51
1	B	176	THR	N-CA-C	5.18	117.59	111.33
1	E	296	ASP	CB-CA-C	-5.13	110.68	116.63
1	K	176	THR	N-CA-C	5.12	117.52	111.33
1	G	116	VAL	N-CA-C	5.12	114.94	107.37
1	C	116	VAL	N-CA-C	5.11	114.93	107.37
1	A	96	ASP	N-CA-C	5.07	117.46	111.33
1	B	171	ALA	N-CA-C	5.06	117.53	111.71
1	J	179	ALA	CA-C-N	5.06	125.09	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	179	ALA	C-N-CA	5.06	125.09	119.32
1	K	52	ILE	N-CA-C	5.06	115.25	108.17
1	D	249	GLY	N-CA-C	5.05	119.80	112.82
1	D	316	ASN	CA-C-N	5.04	125.07	119.32
1	D	316	ASN	C-N-CA	5.04	125.07	119.32
1	I	96	ASP	N-CA-C	5.03	116.76	111.28
1	E	171	ALA	N-CA-C	5.03	116.84	111.36

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	2307	0	2364	20	0
1	B	2310	0	2373	18	0
1	C	2313	0	2377	11	0
1	D	2302	0	2360	21	0
1	E	2313	0	2377	18	0
1	F	2307	0	2364	15	0
1	G	2307	0	2364	11	0
1	H	2315	0	2377	17	0
1	I	2302	0	2360	23	0
1	J	2302	0	2360	21	0
1	K	2310	0	2373	25	0
1	L	2307	0	2364	22	0
2	A	10	0	5	2	0
2	B	10	0	5	0	0
2	C	10	0	5	1	0
2	D	10	0	5	1	0
2	E	10	0	5	1	0
2	F	10	0	5	1	0
2	G	10	0	5	0	0
2	H	10	0	5	1	0
2	I	10	0	5	1	0
2	J	10	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	10	0	5	1	0
2	L	10	0	5	2	0
3	A	7	0	10	5	0
3	B	7	0	10	3	0
3	C	7	0	10	0	0
3	G	7	0	10	0	0
3	K	28	0	40	8	0
4	A	242	0	0	0	0
4	B	191	0	0	0	0
4	C	229	0	0	0	0
4	D	109	0	0	0	0
4	E	146	0	0	0	0
4	F	241	0	0	0	0
4	G	145	0	0	0	0
4	H	129	0	0	0	0
4	I	97	0	0	0	0
4	J	110	0	0	0	0
4	K	148	0	0	1	0
4	L	91	0	0	1	0
All	All	29749	0	28553	206	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 4.

All (206) 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:B:206[A]:ARG:HH11	1:B:206[A]:ARG:HG2	1.05	1.08
1:K:233:MET:HG3	3:K:2001:PEG:H31	1.41	1.01
1:B:233:MET:HG3	3:B:2003:PEG:H22	1.53	0.91
1:B:206[A]:ARG:HG2	1:B:206[A]:ARG:NH1	1.83	0.89
1:A:202:VAL:HG21	3:A:2002:PEG:H12	1.54	0.89
1:A:326:ALA:HB1	3:A:2002:PEG:H11	1.56	0.87
1:D:121:MET:HE1	1:D:168:LYS:HE3	1.68	0.76
1:A:161:GLY:HA3	1:A:166:ILE:HG13	1.68	0.76
1:B:224:TYR:H	3:B:2003:PEG:H41	1.53	0.73
1:J:17:ALA:HA	1:J:39:LEU:HD21	1.71	0.72
1:A:286:PRO:HD2	1:F:192:LYS:HE2	1.71	0.71
1:B:206[A]:ARG:HH11	1:B:206[A]:ARG:CG	1.94	0.71
1:H:283:ILE:HD13	1:H:297:SER:HB3	1.76	0.67
1:I:123:PRO:HG2	1:I:126:ALA:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:224:TYR:H	3:K:2001:PEG:H12	1.63	0.64
1:A:326:ALA:CB	3:A:2002:PEG:H11	2.25	0.63
1:B:17:ALA:HA	1:B:39:LEU:HD11	1.79	0.63
1:L:314:THR:HG22	1:L:316:ASN:H	1.63	0.63
1:E:101:SER:HB2	1:E:102:PRO:HD3	1.79	0.62
1:J:123:PRO:HG2	1:J:126:ALA:HB2	1.80	0.61
1:J:101:SER:HB2	1:J:102:PRO:HD3	1.82	0.61
1:A:133:MET:HE2	1:B:127:ILE:HB	1.83	0.60
3:A:2002:PEG:H22	1:G:231:GLU:OE2	2.00	0.60
1:K:127:ILE:HB	1:L:133:MET:HE2	1.84	0.60
1:E:123:PRO:HG2	1:E:126:ALA:HB2	1.84	0.58
1:L:321:GLN:HE21	1:L:321:GLN:HA	1.66	0.58
1:C:127:ILE:HB	1:D:133:MET:HE2	1.87	0.57
1:K:101:SER:HB2	1:K:102:PRO:HD3	1.86	0.57
1:E:16:ILE:HG21	1:E:92:THR:HB	1.87	0.57
1:B:101:SER:HB2	1:B:102:PRO:HD3	1.88	0.56
1:I:320:ILE:HA	1:I:323:TYR:HD2	1.70	0.56
1:L:283:ILE:HD13	1:L:297:SER:HB3	1.87	0.55
1:G:114:PRO:HD3	1:G:148:ARG:HG2	1.87	0.55
1:C:233:MET:HA	1:C:233:MET:HE2	1.88	0.55
1:I:101:SER:HB2	1:I:102:PRO:HD3	1.87	0.55
1:D:123:PRO:HG2	1:D:126:ALA:HB2	1.88	0.55
1:I:62:SER:OG	2:I:3358:GLU:O	2.24	0.55
1:L:10:LEU:HD13	1:L:89:VAL:HG13	1.90	0.54
1:B:10:LEU:HD13	1:B:89:VAL:HG13	1.89	0.54
1:H:4:LEU:HB3	1:H:50:ALA:HA	1.90	0.54
1:I:4:LEU:HB3	1:I:50:ALA:HA	1.90	0.54
1:F:5:PRO:O	1:F:50:ALA:HB1	2.07	0.53
1:D:320:ILE:HA	1:D:323:TYR:HD1	1.74	0.53
1:C:101:SER:HB2	1:C:102:PRO:HD3	1.90	0.53
1:E:10:LEU:HD13	1:E:89:VAL:HG13	1.91	0.53
1:I:7:ILE:HB	1:I:52:ILE:HG22	1.91	0.53
1:J:133:MET:HE3	1:J:133:MET:HA	1.89	0.52
1:E:264:ARG:HE	1:E:291:PRO:HG3	1.74	0.52
1:D:121:MET:HE1	1:D:168:LYS:CE	2.39	0.52
1:J:228:ASP:HB2	1:L:304:ARG:NH2	2.25	0.51
1:F:66:THR:OG1	1:F:68[A]:ASP:OD2	2.26	0.51
1:D:101:SER:HB2	1:D:102:PRO:HD3	1.92	0.51
1:A:175:ASP:O	1:A:178:LYS:NZ	2.44	0.51
1:J:11:ALA:HA	1:J:92:THR:HB	1.92	0.51
1:K:5:PRO:O	1:K:50:ALA:HB1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:SER:HB2	1:A:94:GLY:HA3	1.93	0.51
1:C:67:SER:OG	1:C:217:LEU:HD12	2.10	0.51
1:D:97:THR:C	1:D:99:ASP:H	2.20	0.50
1:L:260:ASP:OD2	1:L:264:ARG:NH1	2.44	0.50
1:G:67:SER:HB2	1:G:217:LEU:HD12	1.93	0.50
1:G:16:ILE:O	1:G:39:LEU:HD21	2.12	0.50
1:I:56:GLN:NE2	1:I:59:SER:HB2	2.27	0.50
1:J:10:LEU:HD13	1:J:89:VAL:HG13	1.94	0.50
1:D:257:LYS:HG3	1:D:258:ARG:HD3	1.93	0.50
1:L:101:SER:HB2	1:L:102:PRO:HD3	1.93	0.49
1:F:10:LEU:HD13	1:F:89:VAL:HG13	1.94	0.49
1:H:16:ILE:O	1:H:39:LEU:HD21	2.11	0.49
1:J:192:LYS:HD3	1:J:193:ILE:N	2.28	0.49
1:C:39:LEU:HD23	1:C:39:LEU:H	1.77	0.49
1:F:67:SER:HB2	1:F:217:LEU:HD12	1.95	0.49
1:K:4:LEU:HB3	1:K:50:ALA:HA	1.95	0.49
1:H:114:PRO:HD3	1:H:148[A]:ARG:HG2	1.95	0.49
1:K:257:LYS:HB3	1:K:257:LYS:NZ	2.27	0.49
1:B:304:ARG:NH2	1:F:228:ASP:HB2	2.29	0.48
1:K:223:ILE:HA	3:K:2001:PEG:H12	1.95	0.48
1:L:15:THR:OG1	2:L:3361:GLU:HG2	2.13	0.48
1:D:121:MET:HB3	1:D:174:LEU:HD23	1.96	0.47
1:H:10:LEU:HD13	1:H:89:VAL:HG13	1.96	0.47
1:J:114:PRO:HD3	1:J:148:ARG:HG2	1.97	0.47
1:C:283:ILE:HD13	1:C:297:SER:HB3	1.97	0.47
1:A:283:ILE:HD13	1:A:297:SER:HB3	1.95	0.47
1:E:321:GLN:HE21	1:E:321:GLN:HA	1.80	0.47
1:K:304:ARG:HD3	4:K:3371:HOH:O	2.13	0.47
1:A:304:ARG:NH2	1:E:228:ASP:HB2	2.29	0.47
1:G:101:SER:HB2	1:G:102:PRO:HD3	1.97	0.47
1:I:224:TYR:H	3:K:2001:PEG:H11	1.80	0.47
1:C:123:PRO:HG2	1:C:126:ALA:HB2	1.97	0.47
1:F:107:LEU:HD12	1:F:309:LEU:HD12	1.98	0.46
1:D:62:SER:OG	2:D:3355:GLU:O	2.30	0.46
1:A:296:ASP:OD2	1:A:297:SER:N	2.49	0.46
1:L:314:THR:HG22	1:L:315:THR:N	2.30	0.46
1:A:228:ASP:HB2	1:E:304:ARG:NH2	2.30	0.46
1:F:192:LYS:NZ	1:F:192:LYS:HB2	2.31	0.46
1:L:275:ARG:HH12	1:L:290:GLN:NE2	2.13	0.46
1:B:283:ILE:HD13	1:B:297:SER:HB3	1.96	0.46
1:G:283:ILE:HD13	1:G:297:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:56:GLN:HE21	1:I:59:SER:HB2	1.80	0.46
1:H:123:PRO:HG2	1:H:126:ALA:HB2	1.98	0.46
1:I:190:GLY:O	1:I:191:ASP:HB2	2.16	0.46
1:D:313:LYS:HB3	1:D:313:LYS:NZ	2.31	0.46
1:I:122:ARG:NH1	1:I:174:LEU:HD11	2.30	0.46
1:I:319:VAL:HG12	1:I:323:TYR:CE2	2.50	0.46
1:K:145:LYS:HZ2	1:K:145:LYS:H	1.64	0.46
1:A:62:SER:HB3	2:A:3350:GLU:O	2.16	0.46
1:G:5:PRO:O	1:G:50:ALA:HB1	2.15	0.46
1:J:76:ARG:HH21	1:J:80:LEU:HD21	1.81	0.46
1:A:304:ARG:O	1:A:308:MET:HG3	2.15	0.45
1:E:313:LYS:NZ	1:E:313:LYS:HB3	2.31	0.45
1:D:304:ARG:NH2	1:H:228:ASP:HB2	2.31	0.45
1:H:313:LYS:HB3	1:H:313:LYS:NZ	2.31	0.45
1:K:123:PRO:HG2	1:K:126:ALA:HB2	1.98	0.45
1:B:67:SER:HB2	1:B:217:LEU:HD12	1.97	0.45
1:L:62:SER:OG	2:L:3361:GLU:O	2.33	0.45
1:F:4:LEU:HB3	1:F:50:ALA:HA	1.98	0.45
1:J:283:ILE:HD13	1:J:297:SER:HB3	1.99	0.45
1:A:17:ALA:HA	1:A:39:LEU:HD21	1.99	0.45
1:D:113:LYS:HA	1:D:114:PRO:HD3	1.83	0.45
1:B:224:TYR:N	3:B:2003:PEG:H41	2.28	0.45
1:E:62:SER:OG	2:E:3352:GLU:O	2.25	0.44
1:I:228:ASP:HB2	1:K:304:ARG:NH2	2.32	0.44
1:K:206[B]:ARG:HA	3:K:2008:PEG:H22	1.99	0.44
1:H:62:SER:OG	2:H:3357:GLU:O	2.28	0.44
1:K:206[A]:ARG:HA	3:K:2008:PEG:H22	1.99	0.44
1:I:147:SER:HA	1:I:150:ARG:HE	1.82	0.44
1:K:67:SER:HB2	1:K:217:LEU:HD12	1.98	0.44
1:L:62:SER:HB3	1:L:94:GLY:HA3	1.99	0.44
1:E:71:LEU:O	1:E:75[A]:LYS:HG3	2.17	0.44
1:D:247:TYR:CE2	1:D:255:VAL:HG12	2.52	0.44
1:K:296:ASP:OD2	1:K:297:SER:N	2.51	0.44
1:L:140:LYS:HE3	1:L:193:ILE:HG13	1.99	0.44
1:K:233:MET:HG3	3:K:2001:PEG:C3	2.30	0.44
1:B:136:TYR:O	1:B:140:LYS:HB2	2.18	0.44
1:B:206[A]:ARG:NH1	1:B:206[A]:ARG:CG	2.61	0.44
1:D:67:SER:HB2	1:D:217:LEU:HD12	1.98	0.44
1:E:114:PRO:HD3	1:E:148:ARG:HG2	2.00	0.43
1:I:67:SER:HB2	1:I:217:LEU:HD12	1.99	0.43
3:A:2002:PEG:O1	1:G:231:GLU:OE1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:VAL:HG12	1:E:111:SER:H	1.83	0.43
1:J:3:ASN:HD22	1:J:4:LEU:N	2.16	0.43
1:B:5:PRO:O	1:B:50:ALA:HB1	2.19	0.43
1:C:63:GLU:OE1	2:C:3354:GLU:N	2.52	0.43
1:B:110:LYS:NZ	1:B:110:LYS:HB2	2.33	0.43
1:E:314:THR:OG1	1:E:315:THR:N	2.51	0.43
1:D:154:VAL:HG21	1:D:166:ILE:HG21	2.00	0.43
1:J:113:LYS:HA	1:J:114:PRO:HD3	1.91	0.43
1:K:121:MET:HB2	1:K:174:LEU:HD23	2.00	0.43
1:L:137:GLY:O	1:L:141:VAL:HG23	2.18	0.43
1:H:114:PRO:HD3	1:H:148[B]:ARG:HG2	2.00	0.42
1:K:4:LEU:HA	1:K:5:PRO:HD3	1.91	0.42
1:K:320:ILE:HA	1:K:323:TYR:CD2	2.54	0.42
1:H:81:LEU:HD22	1:H:113:LYS:HB2	2.01	0.42
1:J:5:PRO:O	1:J:50:ALA:HB1	2.19	0.42
1:J:109:VAL:HG12	1:J:111:SER:H	1.84	0.42
1:K:109:VAL:HG12	1:K:111:SER:H	1.84	0.42
1:K:145:LYS:HB2	1:K:145:LYS:NZ	2.34	0.42
1:E:321:GLN:HA	1:E:321:GLN:NE2	2.34	0.42
1:D:228:ASP:HB2	1:H:304:ARG:NH2	2.35	0.42
1:D:245:ILE:HB	1:D:273:VAL:HG22	2.02	0.42
1:K:63:GLU:OE1	2:K:3360:GLU:N	2.53	0.42
1:F:283:ILE:HD13	1:F:297:SER:HB3	2.02	0.42
1:K:140:LYS:HE3	1:K:193:ILE:HG13	2.01	0.42
1:L:234:TYR:O	1:L:238:ILE:HG13	2.20	0.42
1:E:137:GLY:O	1:E:141:VAL:HG23	2.19	0.42
1:D:320:ILE:HA	1:D:323:TYR:CD1	2.52	0.42
1:H:320:ILE:HA	1:H:323:TYR:HD1	1.85	0.42
1:I:122:ARG:NH2	1:J:133:MET:HG2	2.34	0.42
1:L:320:ILE:HA	1:L:323:TYR:HD1	1.85	0.42
1:G:113:LYS:HA	1:G:114:PRO:HD3	1.89	0.41
1:I:37:GLU:O	1:I:41:GLN:HG2	2.19	0.41
1:K:202:VAL:HA	3:K:2007:PEG:H21	2.02	0.41
1:A:316:ASN:HA	1:A:317:PRO:HD3	1.86	0.41
1:F:109:VAL:HG12	1:F:111:SER:H	1.85	0.41
1:H:97:THR:C	1:H:99:ASP:H	2.27	0.41
1:F:63:GLU:OE1	2:F:3353:GLU:N	2.52	0.41
1:F:123:PRO:HG2	1:F:126:ALA:HB2	2.02	0.41
1:A:11:ALA:HA	1:A:92:THR:OG1	2.20	0.41
1:D:10:LEU:HD13	1:D:89:VAL:HG13	2.02	0.41
1:G:316:ASN:HA	1:G:317:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:230:PRO:HG2	1:I:233:MET:HG2	2.02	0.41
1:E:113:LYS:HA	1:E:114:PRO:HD3	1.93	0.41
1:L:222:ILE:HG12	1:L:246:VAL:HB	2.03	0.41
1:G:11:ALA:HB2	1:G:36:VAL:HB	2.01	0.41
1:I:133:MET:HE2	1:J:127:ILE:HB	2.02	0.41
1:J:71:LEU:O	1:J:75:LYS:HG3	2.20	0.41
1:J:296:ASP:OD2	1:J:297:SER:N	2.54	0.41
1:J:304:ARG:NH2	1:L:228:ASP:HB2	2.36	0.41
1:H:283:ILE:CD1	1:H:297:SER:HB3	2.47	0.41
1:I:36:VAL:HB	1:I:56:GLN:HB2	2.03	0.41
1:L:321:GLN:HA	1:L:321:GLN:NE2	2.34	0.41
1:A:96:ASP:OD2	2:A:3350:GLU:N	2.54	0.41
1:I:115:VAL:HB	1:I:152:VAL:HG22	2.03	0.41
1:E:283:ILE:HD13	1:E:297:SER:HB3	2.02	0.41
1:F:316:ASN:HA	1:F:317:PRO:HD2	1.91	0.41
1:C:133:MET:HE2	1:D:127:ILE:HB	2.02	0.41
1:C:234:TYR:O	1:C:238:ILE:HG13	2.21	0.41
1:H:109:VAL:HG12	1:H:111:SER:H	1.86	0.41
1:I:293:LEU:HD22	1:I:321:GLN:HB2	2.02	0.41
1:I:113:LYS:HA	1:I:114:PRO:HD3	1.78	0.41
1:L:121:MET:HB2	1:L:174:LEU:HD23	2.02	0.41
1:B:228:ASP:HB2	1:F:304:ARG:NH2	2.36	0.40
1:J:62:SER:OG	2:J:3351:GLU:O	2.31	0.40
1:A:101:SER:HB2	1:A:102:PRO:HD3	2.04	0.40
1:A:137:GLY:O	1:A:141:VAL:HG23	2.22	0.40
1:C:71:LEU:HD11	1:C:217:LEU:HG	2.02	0.40
1:L:304:ARG:HD3	4:L:3442:HOH:O	2.22	0.40
1:H:62:SER:HB2	1:H:97:THR:OG1	2.22	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	305/327 (93%)	300 (98%)	4 (1%)	1 (0%)	36	42
1	B	305/327 (93%)	297 (97%)	7 (2%)	1 (0%)	36	42
1	C	306/327 (94%)	298 (97%)	7 (2%)	1 (0%)	36	42
1	D	304/327 (93%)	296 (97%)	8 (3%)	0	100	100
1	E	306/327 (94%)	299 (98%)	7 (2%)	0	100	100
1	F	305/327 (93%)	299 (98%)	5 (2%)	1 (0%)	36	42
1	G	305/327 (93%)	296 (97%)	9 (3%)	0	100	100
1	H	306/327 (94%)	299 (98%)	7 (2%)	0	100	100
1	I	304/327 (93%)	294 (97%)	10 (3%)	0	100	100
1	J	304/327 (93%)	296 (97%)	8 (3%)	0	100	100
1	K	305/327 (93%)	295 (97%)	9 (3%)	1 (0%)	36	42
1	L	305/327 (93%)	296 (97%)	8 (3%)	1 (0%)	36	42
All	All	3660/3924 (93%)	3565 (97%)	89 (2%)	6 (0%)	43	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	204	THR
1	C	204	THR
1	A	204	THR
1	K	204	THR
1	B	204	THR
1	L	204	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/261 (97%)	252 (100%)	0	100	100
1	B	252/261 (97%)	249 (99%)	3 (1%)	63	78
1	C	253/261 (97%)	252 (100%)	1 (0%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	251/261 (96%)	250 (100%)	1 (0%)	84	92
1	E	253/261 (97%)	252 (100%)	1 (0%)	84	92
1	F	252/261 (97%)	252 (100%)	0	100	100
1	G	252/261 (97%)	252 (100%)	0	100	100
1	H	253/261 (97%)	253 (100%)	0	100	100
1	I	251/261 (96%)	251 (100%)	0	100	100
1	J	251/261 (96%)	251 (100%)	0	100	100
1	K	252/261 (97%)	250 (99%)	2 (1%)	73	85
1	L	252/261 (97%)	252 (100%)	0	100	100
All	All	3024/3132 (97%)	3016 (100%)	8 (0%)	84	93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	76	ARG
1	B	206[A]	ARG
1	B	206[B]	ARG
1	E	313	LYS
1	C	233	MET
1	D	178	LYS
1	K	145	LYS
1	K	257	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	B	3	ASN
1	E	146	ASN
1	E	196	GLN
1	F	196	GLN
1	C	3	ASN
1	C	41	GLN
1	D	290	GLN
1	D	325	HIS
1	G	146	ASN
1	G	196	GLN
1	H	3	ASN

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Mol	Chain	Res	Type
1	H	290	GLN
1	I	3	ASN
1	I	56	GLN
1	I	196	GLN
1	I	213	ASN
1	J	3	ASN
1	K	3	ASN
1	L	3	ASN
1	L	51	ASN
1	L	146	ASN
1	L	290	GLN
1	L	325	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	GLU	G	3356	-	8,9,9	1.08	1 (12%)	8,11,11	1.34	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLU	I	3358	-	8,9,9	1.07	1 (12%)	8,11,11	1.35	1 (12%)
3	PEG	K	2005	-	6,6,6	0.45	0	5,5,5	0.30	0
3	PEG	G	2006	-	6,6,6	0.46	0	5,5,5	0.26	0
3	PEG	C	2004	-	6,6,6	0.45	0	5,5,5	0.28	0
2	GLU	C	3354	-	8,9,9	1.07	1 (12%)	8,11,11	1.31	1 (12%)
2	GLU	F	3353	-	8,9,9	1.08	1 (12%)	8,11,11	1.30	1 (12%)
3	PEG	K	2007	-	6,6,6	0.46	0	5,5,5	0.30	0
3	PEG	A	2002	-	6,6,6	0.48	0	5,5,5	0.18	0
2	GLU	K	3360	-	8,9,9	1.06	1 (12%)	8,11,11	1.35	1 (12%)
2	GLU	B	3359	-	8,9,9	1.09	1 (12%)	8,11,11	1.29	1 (12%)
2	GLU	A	3350	-	8,9,9	1.05	1 (12%)	8,11,11	1.28	1 (12%)
2	GLU	E	3352	-	8,9,9	1.07	1 (12%)	8,11,11	1.32	1 (12%)
2	GLU	D	3355	-	8,9,9	1.06	1 (12%)	8,11,11	1.35	1 (12%)
2	GLU	L	3361	-	8,9,9	1.05	1 (12%)	8,11,11	1.32	1 (12%)
3	PEG	K	2001	-	6,6,6	0.52	0	5,5,5	0.17	0
3	PEG	B	2003	-	6,6,6	0.53	0	5,5,5	0.20	0
2	GLU	H	3357	-	8,9,9	1.05	1 (12%)	8,11,11	1.38	1 (12%)
2	GLU	J	3351	-	8,9,9	1.06	1 (12%)	8,11,11	1.31	1 (12%)
3	PEG	K	2008	-	6,6,6	0.47	0	5,5,5	0.24	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	GLU	G	3356	-	-	6/9/9/9	-
2	GLU	I	3358	-	-	5/9/9/9	-
3	PEG	K	2005	-	-	3/4/4/4	-
3	PEG	G	2006	-	-	3/4/4/4	-
3	PEG	C	2004	-	-	4/4/4/4	-
2	GLU	C	3354	-	-	5/9/9/9	-
2	GLU	F	3353	-	-	4/9/9/9	-
3	PEG	K	2007	-	-	3/4/4/4	-
3	PEG	A	2002	-	-	4/4/4/4	-
2	GLU	K	3360	-	-	9/9/9/9	-
2	GLU	B	3359	-	-	5/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	A	3350	-	-	2/9/9/9	-
2	GLU	E	3352	-	-	5/9/9/9	-
2	GLU	D	3355	-	-	5/9/9/9	-
2	GLU	L	3361	-	-	8/9/9/9	-
3	PEG	K	2001	-	-	1/4/4/4	-
3	PEG	B	2003	-	-	2/4/4/4	-
2	GLU	H	3357	-	-	5/9/9/9	-
2	GLU	J	3351	-	-	4/9/9/9	-
3	PEG	K	2008	-	-	1/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3359	GLU	OXT-C	-2.35	1.23	1.30
2	C	3354	GLU	OXT-C	-2.29	1.23	1.30
2	G	3356	GLU	OXT-C	-2.26	1.23	1.30
2	D	3355	GLU	OXT-C	-2.24	1.23	1.30
2	J	3351	GLU	OXT-C	-2.23	1.23	1.30
2	E	3352	GLU	OXT-C	-2.22	1.23	1.30
2	K	3360	GLU	OXT-C	-2.20	1.23	1.30
2	F	3353	GLU	OXT-C	-2.20	1.23	1.30
2	H	3357	GLU	OXT-C	-2.20	1.23	1.30
2	I	3358	GLU	OXT-C	-2.18	1.23	1.30
2	L	3361	GLU	OXT-C	-2.17	1.23	1.30
2	A	3350	GLU	OXT-C	-2.14	1.23	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3355	GLU	OXT-C-O	-2.84	117.63	124.08
2	K	3360	GLU	OXT-C-O	-2.84	117.64	124.08
2	I	3358	GLU	OXT-C-O	-2.77	117.79	124.08
2	H	3357	GLU	OXT-C-O	-2.75	117.85	124.08
2	G	3356	GLU	OXT-C-O	-2.74	117.86	124.08
2	B	3359	GLU	OXT-C-O	-2.72	117.92	124.08
2	C	3354	GLU	OXT-C-O	-2.72	117.92	124.08
2	E	3352	GLU	OXT-C-O	-2.67	118.01	124.08
2	F	3353	GLU	OXT-C-O	-2.65	118.06	124.08
2	J	3351	GLU	OXT-C-O	-2.64	118.08	124.08
2	A	3350	GLU	OXT-C-O	-2.64	118.09	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	3361	GLU	OXT-C-O	-2.63	118.12	124.08

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	3361	GLU	O-C-CA-N
2	K	3360	GLU	OXT-C-CA-N
2	L	3361	GLU	OXT-C-CA-N
2	D	3355	GLU	OXT-C-CA-N
2	G	3356	GLU	OXT-C-CA-N
3	B	2003	PEG	O1-C1-C2-O2
3	C	2004	PEG	O1-C1-C2-O2
3	A	2002	PEG	O1-C1-C2-O2
3	K	2001	PEG	O2-C3-C4-O4
3	K	2005	PEG	O2-C3-C4-O4
2	B	3359	GLU	OXT-C-CA-N
2	F	3353	GLU	OXT-C-CA-N
2	C	3354	GLU	OXT-C-CA-N
3	A	2002	PEG	O2-C3-C4-O4
2	I	3358	GLU	CA-CB-CG-CD
2	L	3361	GLU	CA-CB-CG-CD
2	A	3350	GLU	OXT-C-CA-N
2	E	3352	GLU	OXT-C-CA-N
2	I	3358	GLU	OXT-C-CA-N
3	K	2007	PEG	O1-C1-C2-O2
3	K	2008	PEG	C1-C2-O2-C3
2	J	3351	GLU	OXT-C-CA-N
3	C	2004	PEG	O2-C3-C4-O4
2	E	3352	GLU	CA-CB-CG-CD
2	A	3350	GLU	O-C-CA-N
2	B	3359	GLU	O-C-CA-N
2	E	3352	GLU	O-C-CA-N
2	F	3353	GLU	O-C-CA-N
2	C	3354	GLU	O-C-CA-N
2	D	3355	GLU	O-C-CA-N
2	G	3356	GLU	O-C-CA-N
2	I	3358	GLU	O-C-CA-N
2	J	3351	GLU	O-C-CA-N
2	K	3360	GLU	O-C-CA-N
3	G	2006	PEG	O2-C3-C4-O4
2	H	3357	GLU	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
3	K	2007	PEG	C4-C3-O2-C2
3	C	2004	PEG	C4-C3-O2-C2
3	G	2006	PEG	C4-C3-O2-C2
3	A	2002	PEG	C1-C2-O2-C3
3	K	2005	PEG	C4-C3-O2-C2
3	K	2007	PEG	C1-C2-O2-C3
3	G	2006	PEG	O1-C1-C2-O2
3	C	2004	PEG	C1-C2-O2-C3
2	K	3360	GLU	N-CA-CB-CG
2	L	3361	GLU	N-CA-CB-CG
3	A	2002	PEG	C4-C3-O2-C2
2	L	3361	GLU	OXT-C-CA-CB
2	L	3361	GLU	O-C-CA-CB
3	B	2003	PEG	C1-C2-O2-C3
2	J	3351	GLU	OE2-CD-CG-CB
2	B	3359	GLU	CA-CB-CG-CD
2	H	3357	GLU	CA-CB-CG-CD
2	J	3351	GLU	OE1-CD-CG-CB
2	G	3356	GLU	OE1-CD-CG-CB
2	L	3361	GLU	OE1-CD-CG-CB
2	H	3357	GLU	O-C-CA-N
2	K	3360	GLU	OE2-CD-CG-CB
2	G	3356	GLU	OE2-CD-CG-CB
2	L	3361	GLU	OE2-CD-CG-CB
2	K	3360	GLU	OE1-CD-CG-CB
2	H	3357	GLU	OE2-CD-CG-CB
2	C	3354	GLU	CA-CB-CG-CD
2	C	3354	GLU	OE2-CD-CG-CB
2	E	3352	GLU	OE2-CD-CG-CB
2	F	3353	GLU	OE2-CD-CG-CB
2	G	3356	GLU	CA-CB-CG-CD
2	K	3360	GLU	CA-CB-CG-CD
2	B	3359	GLU	OE2-CD-CG-CB
2	H	3357	GLU	OE1-CD-CG-CB
2	C	3354	GLU	OE1-CD-CG-CB
2	D	3355	GLU	OE2-CD-CG-CB
2	E	3352	GLU	OE1-CD-CG-CB
2	D	3355	GLU	OE1-CD-CG-CB
2	B	3359	GLU	OE1-CD-CG-CB
2	K	3360	GLU	C-CA-CB-CG
2	K	3360	GLU	O-C-CA-CB
2	F	3353	GLU	OE1-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
2	I	3358	GLU	OE1-CD-CG-CB
2	I	3358	GLU	OE2-CD-CG-CB
2	G	3356	GLU	O-C-CA-CB
2	K	3360	GLU	OXT-C-CA-CB
2	D	3355	GLU	CA-CB-CG-CD
3	K	2005	PEG	O1-C1-C2-O2

There are no ring outliers.

15 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	3358	GLU	1	0
2	C	3354	GLU	1	0
2	F	3353	GLU	1	0
3	K	2007	PEG	1	0
3	A	2002	PEG	5	0
2	K	3360	GLU	1	0
2	A	3350	GLU	2	0
2	E	3352	GLU	1	0
2	D	3355	GLU	1	0
2	L	3361	GLU	2	0
3	K	2001	PEG	5	0
3	B	2003	PEG	3	0
2	H	3357	GLU	1	0
2	J	3351	GLU	1	0
3	K	2008	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	308/327 (94%)	-0.21	6 (1%) 66 63	16, 28, 47, 126	1 (0%)
1	B	308/327 (94%)	-0.03	5 (1%) 70 67	19, 33, 61, 105	1 (0%)
1	C	308/327 (94%)	-0.17	5 (1%) 70 67	14, 30, 51, 91	2 (0%)
1	D	308/327 (94%)	0.48	12 (3%) 43 40	26, 48, 76, 150	0
1	E	308/327 (94%)	0.43	18 (5%) 29 25	22, 41, 72, 143	2 (0%)
1	F	308/327 (94%)	-0.19	6 (1%) 66 63	17, 27, 53, 106	1 (0%)
1	G	308/327 (94%)	0.18	9 (2%) 53 50	18, 38, 70, 124	1 (0%)
1	H	308/327 (94%)	0.35	7 (2%) 61 58	24, 42, 70, 128	2 (0%)
1	I	308/327 (94%)	0.90	44 (14%) 6 4	24, 50, 103, 147	0
1	J	308/327 (94%)	0.68	22 (7%) 22 19	28, 48, 85, 152	0
1	K	308/327 (94%)	0.08	8 (2%) 57 54	22, 35, 73, 114	1 (0%)
1	L	308/327 (94%)	0.77	25 (8%) 18 15	28, 50, 80, 147	1 (0%)
All	All	3696/3924 (94%)	0.27	167 (4%) 38 35	14, 39, 78, 152	12 (0%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	GLY	6.6
1	H	35	GLY	5.0
1	F	36	VAL	4.9
1	C	35	GLY	4.7
1	E	36	VAL	4.6
1	L	15	THR	4.4
1	A	40	ILE	4.4
1	J	39	LEU	4.4
1	C	39	LEU	4.4
1	L	40	ILE	4.2
1	I	36	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	36	VAL	4.0
1	D	39	LEU	4.0
1	D	40	ILE	4.0
1	E	35	GLY	3.9
1	A	39	LEU	3.8
1	K	36	VAL	3.8
1	L	35	GLY	3.8
1	E	40	ILE	3.8
1	H	39	LEU	3.7
1	E	39	LEU	3.6
1	C	36	VAL	3.6
1	J	17	ALA	3.6
1	J	36	VAL	3.5
1	J	16	ILE	3.5
1	J	40	ILE	3.5
1	E	13	GLY	3.4
1	C	3	ASN	3.4
1	B	36	VAL	3.4
1	L	17	ALA	3.4
1	I	8	VAL	3.4
1	I	46	LEU	3.3
1	I	125	THR	3.3
1	I	50	ALA	3.3
1	L	36	VAL	3.3
1	F	35	GLY	3.3
1	K	35	GLY	3.3
1	I	86	VAL	3.3
1	L	16	ILE	3.3
1	I	13	GLY	3.2
1	I	35	GLY	3.2
1	G	40	ILE	3.2
1	D	38	THR	3.2
1	I	48	THR	3.2
1	J	61	GLY	3.2
1	D	37	GLU	3.2
1	I	6	ASN	3.2
1	I	12	THR	3.2
1	G	36	VAL	3.2
1	G	39	LEU	3.1
1	G	35	GLY	3.1
1	A	38	THR	3.0
1	L	38	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	61	GLY	3.0
1	B	35	GLY	3.0
1	I	89	VAL	2.9
1	B	15	THR	2.9
1	F	17	ALA	2.9
1	G	17	ALA	2.9
1	L	39	LEU	2.9
1	E	54	GLY	2.9
1	D	110	LYS	2.9
1	H	17	ALA	2.9
1	I	39	LEU	2.9
1	D	13	GLY	2.8
1	I	40	ILE	2.8
1	I	15	THR	2.8
1	K	15	THR	2.8
1	I	78	ASN	2.8
1	I	74	SER	2.8
1	I	142	ALA	2.8
1	E	17	ALA	2.7
1	I	14	GLY	2.7
1	E	43	VAL	2.7
1	I	214	VAL	2.7
1	L	143	ALA	2.6
1	A	37	GLU	2.6
1	J	15	THR	2.6
1	K	38	THR	2.6
1	L	205	THR	2.6
1	E	60	ILE	2.6
1	I	52	ILE	2.6
1	F	39	LEU	2.6
1	E	38	THR	2.6
1	I	211	VAL	2.6
1	J	35	GLY	2.6
1	J	126	ALA	2.6
1	L	109	VAL	2.6
1	L	292	GLY	2.6
1	L	196	GLN	2.6
1	I	49	LEU	2.6
1	L	111	SER	2.6
1	J	37	GLU	2.5
1	I	215	ASP	2.5
1	I	88	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	38	THR	2.5
1	I	73	LEU	2.5
1	I	38	THR	2.5
1	I	324	PHE	2.5
1	J	323	TYR	2.5
1	E	16	ILE	2.4
1	K	39	LEU	2.4
1	D	17	ALA	2.4
1	I	17	ALA	2.4
1	I	5	PRO	2.4
1	I	42	ALA	2.4
1	G	38	THR	2.4
1	J	125	THR	2.4
1	J	111	SER	2.4
1	F	40	ILE	2.4
1	H	36	VAL	2.4
1	H	60	ILE	2.4
1	I	16	ILE	2.4
1	I	109	VAL	2.4
1	E	37	GLU	2.4
1	I	80	LEU	2.3
1	L	207	SER	2.3
1	I	60	ILE	2.3
1	L	261	ALA	2.3
1	J	49	LEU	2.3
1	D	35	GLY	2.3
1	L	56	GLN	2.3
1	J	9	ILE	2.3
1	L	319	VAL	2.3
1	B	13	GLY	2.2
1	C	17	ALA	2.2
1	K	17	ALA	2.2
1	E	70	LEU	2.2
1	J	8	VAL	2.2
1	I	51	ASN	2.2
1	L	84	SER	2.2
1	G	52	ILE	2.2
1	H	40	ILE	2.2
1	K	49	LEU	2.2
1	B	38	THR	2.2
1	D	15	THR	2.2
1	I	11	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	263	ILE	2.2
1	L	320	ILE	2.2
1	I	87	ASP	2.2
1	L	3	ASN	2.2
1	G	14	GLY	2.2
1	L	219	ALA	2.2
1	J	264	ARG	2.1
1	K	46	LEU	2.1
1	I	3	ASN	2.1
1	I	44	PRO	2.1
1	J	14	GLY	2.1
1	I	82	ALA	2.1
1	L	314	THR	2.1
1	L	4	LEU	2.1
1	J	55	GLU	2.1
1	E	314	THR	2.1
1	J	70	LEU	2.1
1	I	77	VAL	2.1
1	J	5	PRO	2.1
1	G	59	SER	2.1
1	H	42	ALA	2.1
1	F	16	ILE	2.1
1	I	141	VAL	2.1
1	D	59	SER	2.0
1	I	129	ALA	2.0
1	A	36	VAL	2.0
1	E	14	GLY	2.0
1	L	110	LYS	2.0
1	E	41	GLN	2.0
1	E	80	LEU	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

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
3	PEG	C	2004	7/7	0.69	0.17	43,64,78,82	0
3	PEG	K	2008	7/7	0.69	0.18	59,64,71,73	0
3	PEG	G	2006	7/7	0.71	0.17	36,53,65,68	0
3	PEG	K	2007	7/7	0.77	0.15	59,73,81,83	0
3	PEG	K	2005	7/7	0.77	0.14	58,66,70,72	0
2	GLU	L	3361	10/10	0.80	0.15	40,50,62,70	0
2	GLU	J	3351	10/10	0.81	0.13	59,63,69,70	0
3	PEG	B	2003	7/7	0.83	0.21	10,24,48,58	0
3	PEG	K	2001	7/7	0.84	0.18	16,26,47,57	0
2	GLU	H	3357	10/10	0.84	0.11	46,52,61,75	0
2	GLU	I	3358	10/10	0.84	0.12	38,44,54,56	0
3	PEG	A	2002	7/7	0.84	0.19	19,38,50,59	0
2	GLU	E	3352	10/10	0.87	0.11	36,44,55,59	0
2	GLU	D	3355	10/10	0.87	0.08	40,43,57,57	0
2	GLU	K	3360	10/10	0.89	0.09	29,37,53,57	0
2	GLU	G	3356	10/10	0.92	0.08	33,41,50,60	0
2	GLU	F	3353	10/10	0.92	0.10	24,38,43,45	0
2	GLU	C	3354	10/10	0.94	0.08	28,34,39,52	0
2	GLU	A	3350	10/10	0.94	0.07	23,32,39,40	0
2	GLU	B	3359	10/10	0.95	0.08	27,28,49,52	0

6.5 Other polymers

There are no such residues in this entry.