Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:34 AM GMT

PDB ID	:	2HLN
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

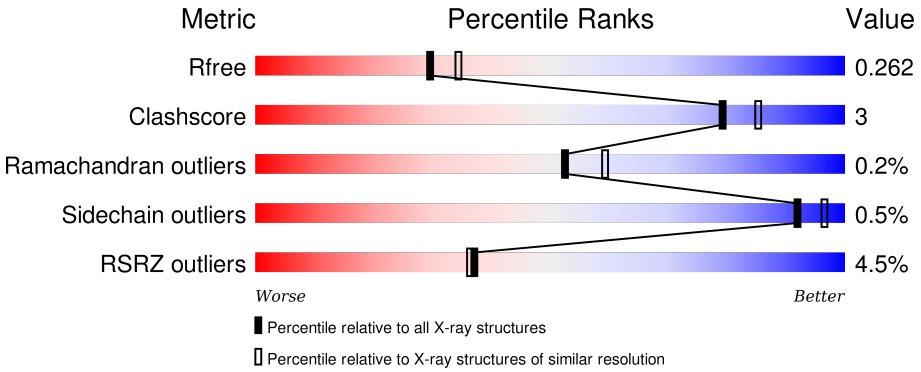
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	2% 86% 8% 6%
1	B	327	2% 87% 7% 6%
1	C	327	2% 90% • 6%
1	D	327	4% 85% 8% • 6%
1	E	327	4% 86% 8% 6%

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Mol	Chain	Length	Quality of chain
1	F	327	2% 87% 7% 6%
1	G	327	4% 89% 6% 6%
1	H	327	3% 87% 7% 6%
1	I	327	11% 83% 11% 6%
1	J	327	7% 84% 9% 6%
1	K	327	3% 85% 8% 6%
1	L	327	6% 84% 9% 6%

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	X
3	PEG	B	2003	-	-	-	X
3	PEG	C	2004	-	-	-	X
3	PEG	G	2006	-	-	-	X
3	PEG	K	2001	-	-	X	X
3	PEG	K	2005	-	-	-	X

2 Entry composition (i)

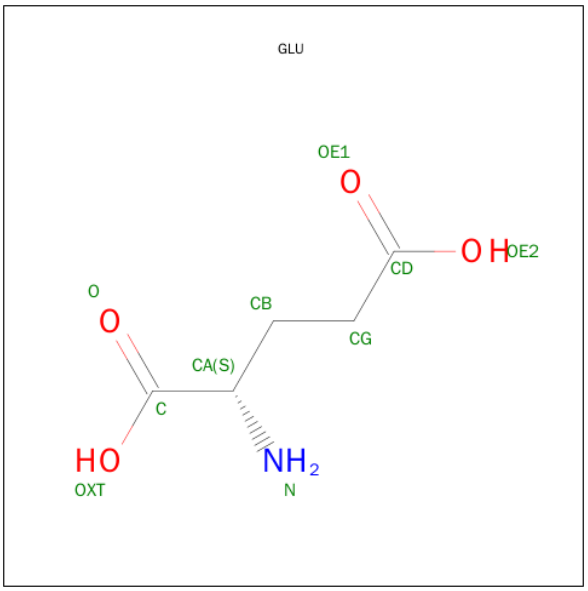
There are 4 unique types of molecules in this entry. The entry contains 29749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

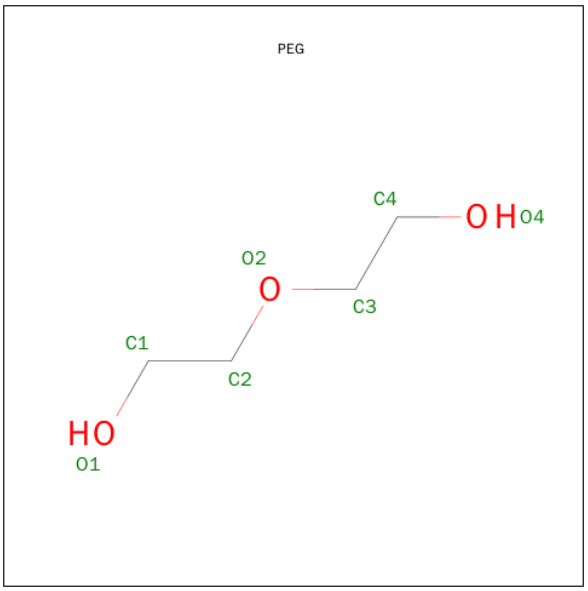
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	1	0
			2307	1456	395	450	6			
1	B	308	Total	C	N	O	S	0	1	0
			2310	1458	398	448	6			
1	E	308	Total	C	N	O	S	0	2	0
			2313	1461	396	450	6			
1	F	308	Total	C	N	O	S	0	1	0
			2307	1456	395	450	6			
1	C	308	Total	C	N	O	S	0	2	0
			2313	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 (three-letter code: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	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	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	B	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 (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- 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	C	229	Total O 229 229	0	0
4	D	109	Total O 109 109	0	0

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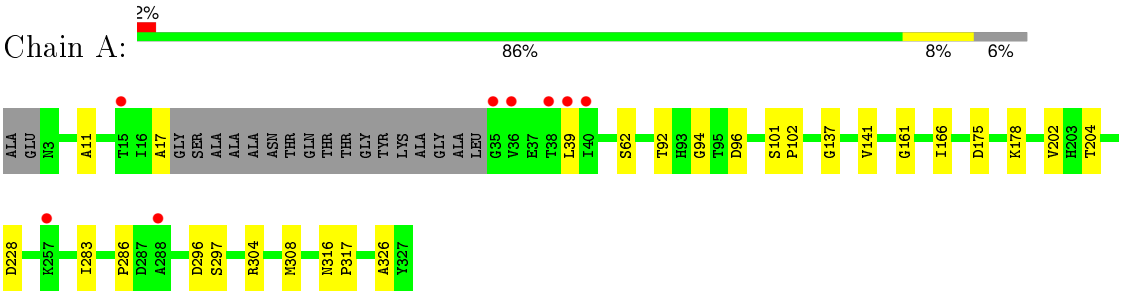
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	146	Total O 146 146	0	0
4	F	241	Total O 241 241	0	0
4	G	145	Total O 145 145	0	0
4	H	129	Total O 129 129	0	0
4	I	97	Total O 97 97	0	0
4	J	110	Total O 110 110	0	0
4	K	148	Total O 148 148	0	0
4	L	91	Total O 91 91	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

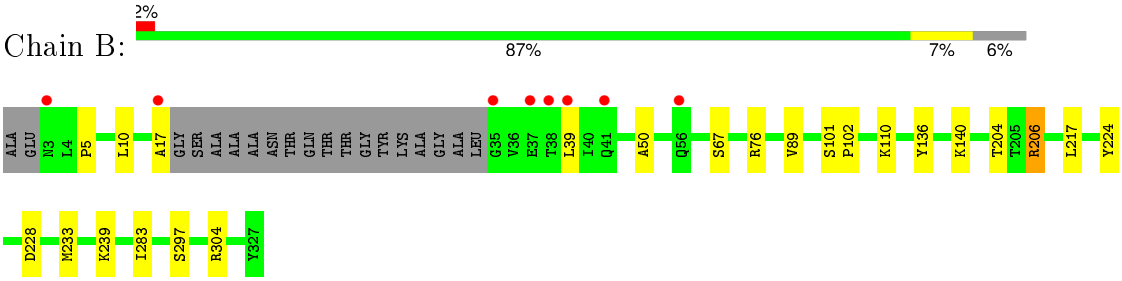
- Molecule 1: L-asparaginase

Chain A:



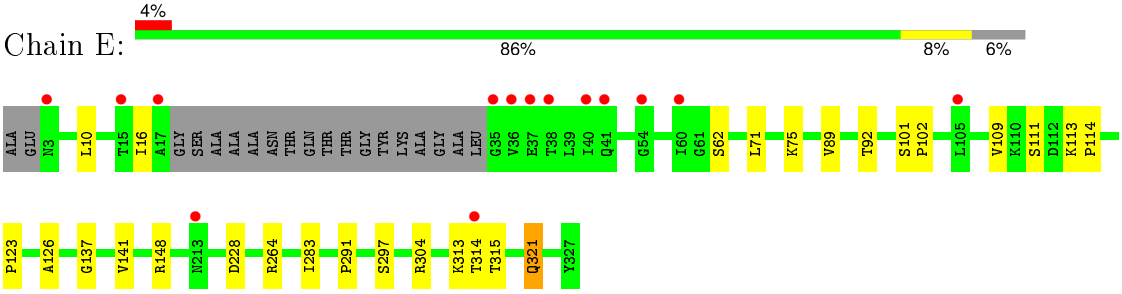
- Molecule 1: L-asparaginase

Chain B:



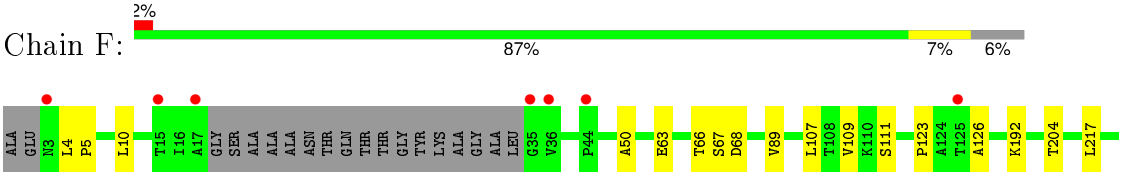
- Molecule 1: L-asparaginase

Chain E:



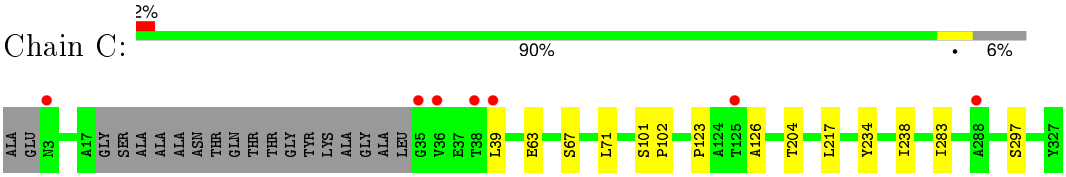
- Molecule 1: L-asparaginase

Chain F:



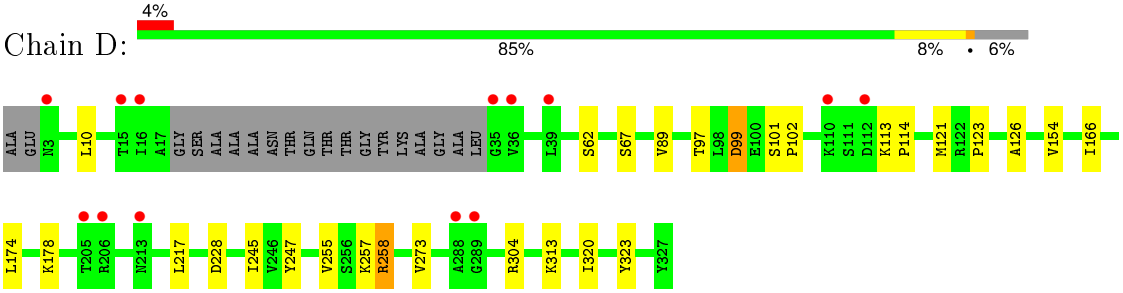
• Molecule 1: L-asparaginase

Chain C:



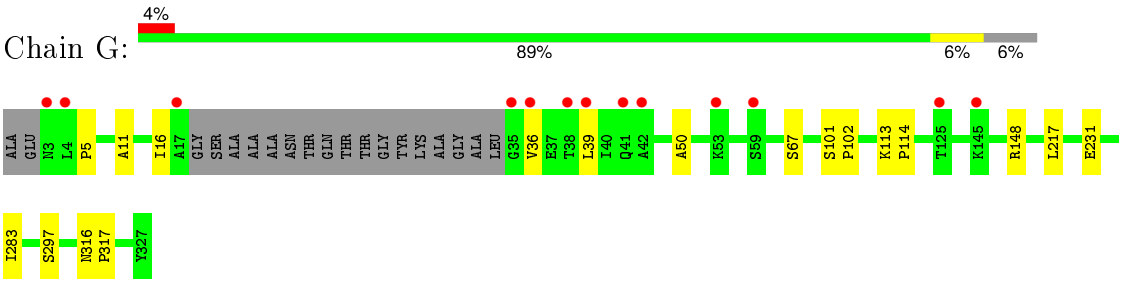
• Molecule 1: L-asparaginase

Chain D:



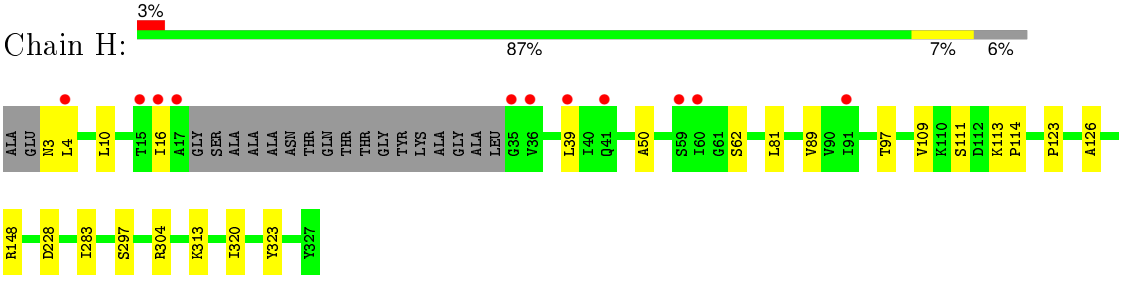
• Molecule 1: L-asparaginase

Chain G:



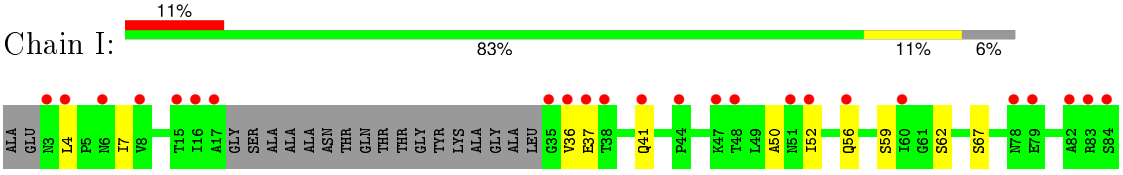
• Molecule 1: L-asparaginase

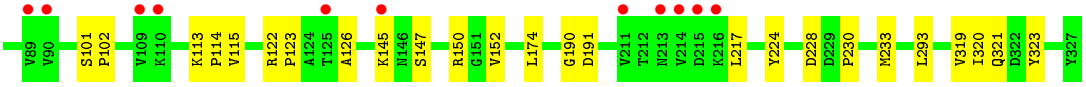
Chain H:



• Molecule 1: L-asparaginase

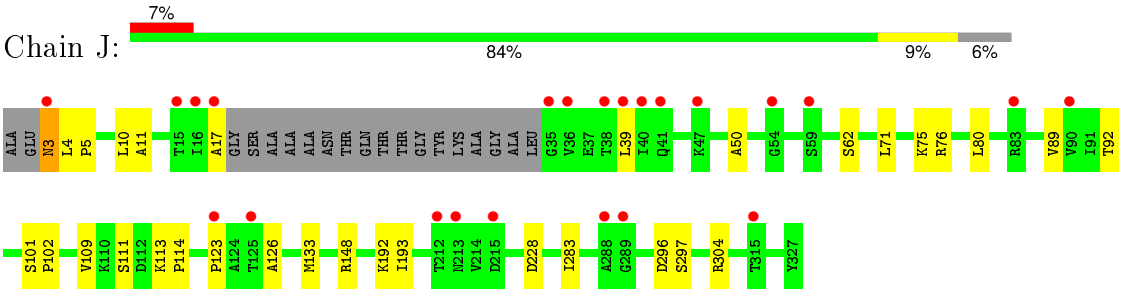
Chain I:





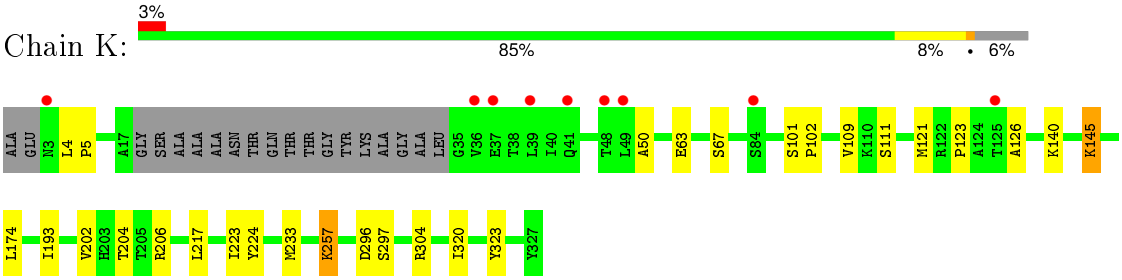
• Molecule 1: L-asparaginase

Chain J:



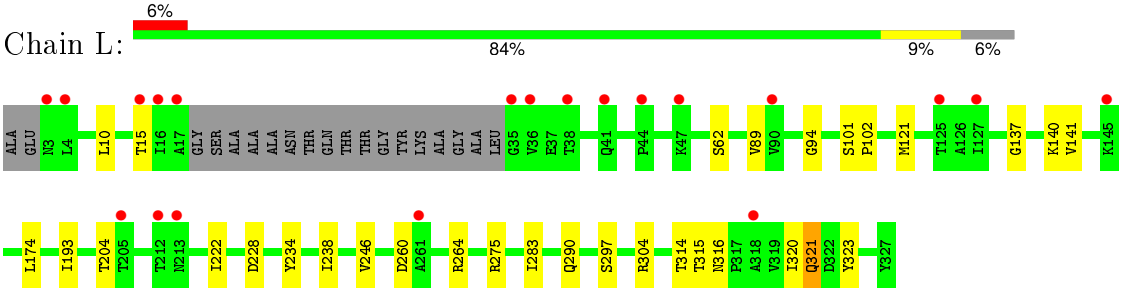
• Molecule 1: L-asparaginase

Chain K:



• Molecule 1: L-asparaginase

Chain L:



4 Data and refinement statistics (i)

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) 91.1 (19.98-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.29%)	DCC
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.2	EDS
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	3 of 179501 reflections (0.002%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.27	0/2344	0.50	0/3181
1	B	0.27	0/2347	0.50	0/3184
1	C	0.28	0/2353	0.50	0/3192
1	D	0.26	0/2336	0.47	0/3170
1	E	0.27	0/2353	0.48	0/3192
1	F	0.28	0/2344	0.50	0/3181
1	G	0.26	0/2344	0.48	0/3181
1	H	0.26	0/2355	0.48	0/3195
1	I	0.26	0/2336	0.48	0/3170
1	J	0.26	0/2336	0.48	0/3170
1	K	0.27	0/2347	0.48	0/3184
1	L	0.26	0/2344	0.47	0/3181
All	All	0.27	0/28139	0.49	0/38181

There are no bond length outliers.

There are no bond angle outliers.

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	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2310	0	2373	17	0
1	C	2313	0	2377	8	0
1	D	2302	0	2360	17	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	16	0
1	I	2302	0	2360	22	0
1	J	2302	0	2360	19	0
1	K	2310	0	2373	24	0
1	L	2307	0	2364	20	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
2	K	10	0	5	1	0
2	L	10	0	5	1	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	195	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 3.

All (195) 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: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
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
3:A:2002:PEG:H22	1:G:231:GLU:OE2	2.00	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:264:ARG:HE	1:E:291:PRO:HG3	1.74	0.52
1:J:228:ASP:HB2	1:L:304:ARG:NH2	2.25	0.51
1:D:101:SER:HB2	1:D:102:PRO:HD3	1.92	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
1:A:175:ASP:O	1:A:178:LYS:NZ	2.44	0.51
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: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:J:10:LEU:HD13	1:J:89:VAL:HG13	1.94	0.50
1:I:56:GLN:NE2	1:I:59:SER:HB2	2.27	0.50
1:G:16:ILE:O	1:G:39:LEU:HD21	2.12	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:H	1:C:39:LEU:HD23	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:NZ	1:K:257:LYS:HB3	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:J:114:PRO:HD3	1:J:148:ARG:HG2	1.97	0.47
1:H:10:LEU:HD13	1:H:89:VAL:HG13	1.96	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:HA	1:E:321:GLN:HE21	1.80	0.47
1:K:304:ARG:HD3	4:K:3371:HOH:O	2.13	0.47
1:I:224:TYR:H	3:K:2001:PEG:H11	1.80	0.47
1:G:101:SER:HB2	1:G:102:PRO:HD3	1.97	0.47
1:A:304:ARG:NH2	1:E:228:ASP:HB2	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:SER:OG	2:D:3355:GLU:O	2.30	0.46
1:L:314:THR:HG22	1:L:315:THR:N	2.30	0.46
1:A:296:ASP:OD2	1:A:297:SER:N	2.49	0.46
1:F:192:LYS:NZ	1:F:192:LYS:HB2	2.31	0.46
1:A:228:ASP:HB2	1:E:304:ARG:NH2	2.30	0.46
1:L:275:ARG:HH12	1:L:290:GLN:NE2	2.13	0.46
1:I:56:GLN:HE21	1:I:59:SER:HB2	1.80	0.46
1:G:283:ILE:HD13	1:G:297:SER:HB3	1.98	0.46
1:B:283:ILE:HD13	1:B:297:SER:HB3	1.96	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:I:122:ARG:NH1	1:I:174:LEU:HD11	2.30	0.46
1:D:313:LYS:NZ	1:D:313:LYS:HB3	2.31	0.46
1:I:319:VAL:HG12	1:I:323:TYR:CE2	2.50	0.46
1:A:62:SER:HB3	2:A:3350:GLU:O	2.16	0.46
1:D:97:THR:C	1:D:99:ASP:H	2.20	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:H:313:LYS:HB3	1:H:313:LYS:NZ	2.31	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:E:62:SER:OG	2:E:3352:GLU:O	2.25	0.45
1:K:123:PRO:HG2	1:K:126:ALA:HB2	1.98	0.45
3:A:2002:PEG:O1	1:G:231:GLU:OE1	2.34	0.45
1:B:67:SER:HB2	1:B:217:LEU:HD12	1.97	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:D:113:LYS:HA	1:D:114:PRO:HD3	1.83	0.45
1:A:17:ALA:HA	1:A:39:LEU:HD21	1.99	0.45
1:B:224:TYR:N	3:B:2003:PEG:H41	2.28	0.45
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:L:62:SER:HB3	1:L:94:GLY:HA3	1.99	0.44
1:K:67:SER:HB2	1:K:217:LEU:HD12	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:LEU:O	1:E:75[A]:LYS:HG3	2.17	0.44
1:K:233:MET:HG3	3:K:2001:PEG:C3	2.30	0.44
1:B:206[A]:ARG:NH1	1:B:206[A]:ARG:CG	2.61	0.44
1:B:136:TYR:O	1:B:140:LYS:HB2	2.18	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
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:J:113:LYS:HA	1:J:114:PRO:HD3	1.91	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:B:110:LYS:HB2	1:B:110:LYS:NZ	2.33	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:K:4:LEU:HA	1:K:5:PRO:HD3	1.91	0.42
1:H:114:PRO:HD3	1:H:148[B]:ARG:HG2	2.00	0.42
1:K:320:ILE:HA	1:K:323:TYR:CD2	2.54	0.42
1:K:145:LYS:NZ	1:K:145:LYS:HB2	2.34	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:E:321:GLN:HA	1:E:321:GLN:NE2	2.34	0.42
1:D:245:ILE:HB	1:D:273:VAL:HG22	2.02	0.42
1:D:228:ASP:HB2	1:H:304:ARG:NH2	2.35	0.42
1:K:63:GLU:OE1	2:K:3360:GLU:N	2.53	0.42
1:K:140:LYS:HE3	1:K:193:ILE:HG13	2.01	0.42
1:F:283:ILE:HD13	1:F:297:SER:HB3	2.02	0.42
1:K:145:LYS:HB2	1:K:145:LYS:HZ3	1.84	0.42
1:L:234:TYR:O	1:L:238:ILE:HG13	2.20	0.42
1:D:320:ILE:HA	1:D:323:TYR:CD1	2.52	0.42
1:I:122:ARG:NH2	1:J:133:MET:HG2	2.34	0.42
1:E:137:GLY:O	1:E:141:VAL:HG23	2.19	0.42
1:H:320:ILE:HA	1:H:323:TYR:HD1	1.85	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:K:202:VAL:HA	3:K:2007:PEG:H21	2.02	0.41
1:I:37:GLU:O	1:I:41:GLN:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:VAL:HG12	1:F:111:SER:H	1.85	0.41
1:A:316:ASN:HA	1:A:317:PRO:HD3	1.86	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:G:316:ASN:HA	1:G:317:PRO:HD3	1.90	0.41
1:A:11:ALA:HA	1:A:92:THR:OG1	2.20	0.41
1:I:230:PRO:HG2	1:I:233:MET:HG2	2.02	0.41
1:D:10:LEU:HD13	1:D:89:VAL:HG13	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:J:296:ASP:OD2	1:J:297:SER:N	2.54	0.41
1:J:71:LEU:O	1:J:75:LYS:HG3	2.20	0.41
1:J:304:ARG:NH2	1:L:228:ASP:HB2	2.36	0.41
1:G:11:ALA:HB2	1:G:36:VAL:HB	2.01	0.41
1:H:283:ILE:CD1	1:H:297:SER:HB3	2.47	0.41
1:L:321:GLN:NE2	1:L:321:GLN:HA	2.34	0.41
1:I:36:VAL:HB	1:I:56:GLN:HB2	2.03	0.41
1:A:96:ASP:OD2	2:A:3350:GLU:N	2.54	0.41
1:F:66:THR:OG1	1:F:68[A]:ASP:OD2	2.26	0.41
1:I:115:VAL:HB	1:I:152:VAL:HG22	2.03	0.41
1:I:293:LEU:HD22	1:I:321:GLN:HB2	2.02	0.41
1:F:316:ASN:HA	1:F:317:PRO:HD2	1.91	0.41
1:H:109:VAL:HG12	1:H:111:SER:H	1.86	0.41
1:E:283:ILE:HD13	1:E:297:SER:HB3	2.02	0.41
1:C:234:TYR:O	1:C:238:ILE:HG13	2.21	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:C:71:LEU:HD11	1:C:217:LEU:HG	2.02	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: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

5.3.1 Protein backbone

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%)	46	50
1	B	305/327 (93%)	297 (97%)	7 (2%)	1 (0%)	46	50
1	C	306/327 (94%)	298 (97%)	7 (2%)	1 (0%)	46	50
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%)	46	50
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%)	46	50
1	L	305/327 (93%)	296 (97%)	8 (3%)	1 (0%)	46	50
All	All	3660/3924 (93%)	3565 (97%)	89 (2%)	6 (0%)	52	59

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%)	248 (98%)	4 (2%)	70 82
1	C	253/261 (97%)	253 (100%)	0	100 100
1	D	251/261 (96%)	248 (99%)	3 (1%)	78 88
1	E	253/261 (97%)	252 (100%)	1 (0%)	93 97
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%)	252 (100%)	1 (0%)	93 97
1	I	251/261 (96%)	250 (100%)	1 (0%)	93 97
1	J	251/261 (96%)	250 (100%)	1 (0%)	93 97
1	K	252/261 (97%)	250 (99%)	2 (1%)	86 93
1	L	252/261 (97%)	251 (100%)	1 (0%)	93 97
All	All	3024/3132 (97%)	3010 (100%)	14 (0%)	92 96

All (14) 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	B	239	LYS
1	E	321	GLN
1	D	99	ASP
1	D	178	LYS
1	D	258	ARG
1	H	3	ASN
1	I	145	LYS
1	J	3	ASN
1	K	145	LYS
1	K	257	LYS
1	L	321	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	B	3	ASN
1	E	146	ASN
1	E	325	HIS
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
1	I	3	ASN
1	I	196	GLN
1	I	213	ASN
1	J	3	ASN
1	K	3	ASN
1	L	3	ASN
1	L	146	ASN
1	L	290	GLN
1	L	325	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	PEG	A	2002	-	6,6,6	0.47	0	5,5,5	0.19	0
2	GLU	A	3350	-	3,9,9	0.09	0	2,11,11	0.52	0
3	PEG	B	2003	-	6,6,6	0.52	0	5,5,5	0.21	0
2	GLU	B	3359	-	3,9,9	0.05	0	2,11,11	0.53	0
3	PEG	C	2004	-	6,6,6	0.44	0	5,5,5	0.31	0
2	GLU	C	3354	-	3,9,9	0.09	0	2,11,11	0.59	0
2	GLU	D	3355	-	3,9,9	0.10	0	2,11,11	0.53	0
2	GLU	E	3352	-	3,9,9	0.11	0	2,11,11	0.60	0
2	GLU	F	3353	-	3,9,9	0.10	0	2,11,11	0.67	0
3	PEG	G	2006	-	6,6,6	0.45	0	5,5,5	0.29	0
2	GLU	G	3356	-	3,9,9	0.11	0	2,11,11	0.58	0
2	GLU	H	3357	-	3,9,9	0.11	0	2,11,11	0.57	0
2	GLU	I	3358	-	3,9,9	0.10	0	2,11,11	0.59	0
2	GLU	J	3351	-	3,9,9	0.10	0	2,11,11	0.54	0
3	PEG	K	2001	-	6,6,6	0.51	0	5,5,5	0.19	0
3	PEG	K	2005	-	6,6,6	0.44	0	5,5,5	0.32	0
3	PEG	K	2007	-	6,6,6	0.45	0	5,5,5	0.31	0
3	PEG	K	2008	-	6,6,6	0.46	0	5,5,5	0.26	0
2	GLU	K	3360	-	3,9,9	0.09	0	2,11,11	0.64	0
2	GLU	L	3361	-	3,9,9	0.10	0	2,11,11	0.54	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
3	PEG	A	2002	-	-	0/4/4/4	0/0/0/0
2	GLU	A	3350	-	-	0/3/9/9	0/0/0/0
3	PEG	B	2003	-	-	0/4/4/4	0/0/0/0
2	GLU	B	3359	-	-	0/3/9/9	0/0/0/0
3	PEG	C	2004	-	-	0/4/4/4	0/0/0/0
2	GLU	C	3354	-	-	0/3/9/9	0/0/0/0
2	GLU	D	3355	-	-	0/3/9/9	0/0/0/0
2	GLU	E	3352	-	-	0/3/9/9	0/0/0/0
2	GLU	F	3353	-	-	0/3/9/9	0/0/0/0
3	PEG	G	2006	-	-	0/4/4/4	0/0/0/0
2	GLU	G	3356	-	-	0/3/9/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	H	3357	-	-	0/3/9/9	0/0/0/0
2	GLU	I	3358	-	-	0/3/9/9	0/0/0/0
2	GLU	J	3351	-	-	0/3/9/9	0/0/0/0
3	PEG	K	2001	-	-	0/4/4/4	0/0/0/0
3	PEG	K	2005	-	-	0/4/4/4	0/0/0/0
3	PEG	K	2007	-	-	0/4/4/4	0/0/0/0
3	PEG	K	2008	-	-	0/4/4/4	0/0/0/0
2	GLU	K	3360	-	-	0/3/9/9	0/0/0/0
2	GLU	L	3361	-	-	0/3/9/9	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2002	PEG	5	0
2	A	3350	GLU	2	0
3	B	2003	PEG	3	0
2	C	3354	GLU	1	0
2	D	3355	GLU	1	0
2	E	3352	GLU	1	0
2	F	3353	GLU	1	0
2	H	3357	GLU	1	0
2	I	3358	GLU	1	0
2	J	3351	GLU	1	0
3	K	2001	PEG	5	0
3	K	2007	PEG	1	0
3	K	2008	PEG	2	0
2	K	3360	GLU	1	0
2	L	3361	GLU	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	308/327 (94%)	-0.35	8 (2%) 59 58	17, 28, 47, 126	0
1	B	308/327 (94%)	-0.24	8 (2%) 59 58	19, 33, 61, 105	0
1	C	308/327 (94%)	-0.34	7 (2%) 64 63	19, 30, 51, 91	0
1	D	308/327 (94%)	0.21	13 (4%) 40 39	26, 48, 76, 150	0
1	E	308/327 (94%)	0.16	14 (4%) 37 36	22, 41, 72, 143	0
1	F	308/327 (94%)	-0.39	7 (2%) 64 63	17, 28, 53, 106	0
1	G	308/327 (94%)	-0.08	13 (4%) 40 39	18, 38, 70, 124	0
1	H	308/327 (94%)	0.01	11 (3%) 46 45	26, 42, 70, 128	0
1	I	308/327 (94%)	0.59	35 (11%) 7 6	24, 50, 103, 147	0
1	J	308/327 (94%)	0.30	23 (7%) 17 17	28, 48, 85, 152	0
1	K	308/327 (94%)	-0.15	9 (2%) 55 54	22, 35, 73, 114	0
1	L	308/327 (94%)	0.46	20 (6%) 22 22	28, 50, 80, 147	0
All	All	3696/3924 (94%)	0.02	168 (4%) 37 36	17, 39, 78, 152	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	35	GLY	12.6
1	I	35	GLY	11.2
1	E	35	GLY	10.6
1	J	36	VAL	8.2
1	D	36	VAL	7.3
1	I	36	VAL	7.1
1	L	16	ILE	7.1
1	J	35	GLY	6.6
1	L	35	GLY	6.5
1	J	39	LEU	6.1
1	D	39	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	17	ALA	5.6
1	K	3	ASN	5.6
1	L	3	ASN	5.6
1	E	36	VAL	5.5
1	D	288	ALA	5.4
1	I	213	ASN	5.3
1	L	15	THR	5.2
1	I	47	LYS	5.0
1	I	17	ALA	5.0
1	B	35	GLY	4.9
1	A	35	GLY	4.9
1	I	84	SER	4.8
1	J	125	THR	4.8
1	C	39	LEU	4.7
1	D	3	ASN	4.6
1	A	38	THR	4.6
1	H	39	LEU	4.3
1	F	36	VAL	4.3
1	I	38	THR	4.3
1	L	36	VAL	4.3
1	J	15	THR	4.2
1	E	41	GLN	4.1
1	I	3	ASN	4.0
1	H	41	GLN	3.9
1	L	205	THR	3.9
1	J	38	THR	3.8
1	D	110	LYS	3.7
1	B	3	ASN	3.7
1	I	215	ASP	3.7
1	I	125	THR	3.7
1	C	36	VAL	3.6
1	H	35	GLY	3.6
1	I	48	THR	3.6
1	J	16	ILE	3.5
1	G	3	ASN	3.5
1	A	36	VAL	3.5
1	J	213	ASN	3.5
1	A	39	LEU	3.5
1	G	125	THR	3.5
1	I	90	VAL	3.4
1	L	17	ALA	3.3
1	E	3	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	59	SER	3.3
1	H	4	LEU	3.3
1	A	40	ILE	3.3
1	L	213	ASN	3.2
1	I	82	ALA	3.2
1	J	54	GLY	3.2
1	G	39	LEU	3.2
1	L	318	ALA	3.2
1	H	59	SER	3.2
1	H	15	THR	3.2
1	I	51	ASN	3.2
1	C	35	GLY	3.2
1	G	41	GLN	3.1
1	D	206	ARG	3.1
1	G	17	ALA	3.1
1	L	41	GLN	3.0
1	L	90	VAL	3.0
1	I	145	LYS	3.0
1	I	216	LYS	3.0
1	K	36	VAL	3.0
1	I	15	THR	3.0
1	F	15	THR	2.9
1	D	213	ASN	2.9
1	H	17	ALA	2.9
1	E	213	ASN	2.9
1	I	79	GLU	2.9
1	E	54	GLY	2.9
1	D	289	GLY	2.9
1	K	125	THR	2.9
1	F	3	ASN	2.9
1	E	60	ILE	2.8
1	C	3	ASN	2.8
1	J	3	ASN	2.8
1	I	4	LEU	2.8
1	C	38	THR	2.8
1	G	38	THR	2.8
1	G	35	GLY	2.7
1	L	125	THR	2.7
1	I	214	VAL	2.7
1	L	145	LYS	2.6
1	E	38	THR	2.6
1	F	125	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	39	LEU	2.6
1	B	17	ALA	2.6
1	J	47	LYS	2.6
1	I	6	ASN	2.6
1	I	16	ILE	2.6
1	L	212	THR	2.5
1	I	52	ILE	2.5
1	I	83	ARG	2.5
1	K	49	LEU	2.5
1	E	105	LEU	2.5
1	I	37	GLU	2.5
1	F	44	PRO	2.5
1	G	42	ALA	2.5
1	J	212	THR	2.4
1	F	17	ALA	2.4
1	I	60	ILE	2.4
1	H	60	ILE	2.4
1	K	41	GLN	2.4
1	J	289	GLY	2.4
1	I	56	GLN	2.4
1	I	211	VAL	2.4
1	A	15	THR	2.4
1	J	315	THR	2.4
1	G	145	LYS	2.4
1	D	15	THR	2.3
1	I	44	PRO	2.3
1	B	38	THR	2.3
1	B	37	GLU	2.3
1	H	91	ILE	2.3
1	I	8	VAL	2.3
1	J	40	ILE	2.3
1	E	314	THR	2.3
1	E	37	GLU	2.3
1	A	288	ALA	2.3
1	L	38	THR	2.3
1	B	56	GLN	2.2
1	I	41	GLN	2.2
1	L	4	LEU	2.2
1	E	40	ILE	2.2
1	L	261	ALA	2.2
1	E	15	THR	2.2
1	J	17	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	16	ILE	2.2
1	L	127	ILE	2.2
1	F	35	GLY	2.2
1	D	205	THR	2.2
1	G	59	SER	2.2
1	I	109	VAL	2.2
1	D	112	ASP	2.2
1	A	257	LYS	2.1
1	B	41	GLN	2.1
1	J	41	GLN	2.1
1	H	36	VAL	2.1
1	K	48	THR	2.1
1	G	36	VAL	2.1
1	C	125	THR	2.1
1	C	288	ALA	2.1
1	G	53	LYS	2.1
1	J	215	ASP	2.1
1	I	110	LYS	2.1
1	L	47	LYS	2.1
1	K	39	LEU	2.1
1	K	84	SER	2.1
1	H	16	ILE	2.1
1	J	90	VAL	2.1
1	K	37	GLU	2.0
1	I	78	ASN	2.0
1	J	83	ARG	2.0
1	J	123	PRO	2.0
1	L	44	PRO	2.0
1	I	89	VAL	2.0
1	J	288	ALA	2.0
1	G	4	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	PEG	A	2002	7/7	0.88	0.21	8.12	19,38,50,59	0
3	PEG	K	2005	7/7	0.76	0.27	5.50	58,66,70,72	0
3	PEG	G	2006	7/7	0.75	0.22	5.24	36,53,65,68	0
3	PEG	K	2001	7/7	0.79	0.22	3.87	16,26,47,57	0
3	PEG	C	2004	7/7	0.83	0.21	2.21	43,64,78,82	0
3	PEG	B	2003	7/7	0.88	0.20	2.00	10,24,48,58	0
3	PEG	K	2007	7/7	0.77	0.26	1.56	59,73,81,83	0
3	PEG	K	2008	7/7	0.69	0.24	1.27	59,64,71,73	0
2	GLU	L	3361	10/10	0.82	0.18	0.49	40,50,62,70	0
2	GLU	H	3357	10/10	0.90	0.17	0.36	46,52,61,75	0
2	GLU	J	3351	10/10	0.82	0.17	0.06	59,63,69,70	0
2	GLU	F	3353	10/10	0.94	0.12	0.05	24,38,43,45	0
2	GLU	A	3350	10/10	0.96	0.10	-0.13	23,32,39,40	0
2	GLU	E	3352	10/10	0.90	0.13	-0.33	36,44,55,59	0
2	GLU	D	3355	10/10	0.94	0.11	-0.46	40,43,57,57	0
2	GLU	I	3358	10/10	0.90	0.12	-0.62	38,44,54,56	0
2	GLU	G	3356	10/10	0.97	0.10	-0.65	33,41,50,60	0
2	GLU	C	3354	10/10	0.96	0.09	-0.66	28,34,39,52	0
2	GLU	B	3359	10/10	0.95	0.10	-0.68	27,28,49,52	0
2	GLU	K	3360	10/10	0.95	0.09	-0.92	29,37,53,57	0

6.5 Other polymers (i)

There are no such residues in this entry.