

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	2HLN
Title	:	L-asparaginase from Erwinia carotovora in complex with glutamic acid
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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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	А	327	86%	8%	6%
1	В	327	2% 87 %	7%	6%
1	С	327	2% 90%	•	6%
1	D	327	4% 85%	8%	6%
1	Е	327	4% 86%	8%	6%



001000	nucu jion	i precious	puge	
Mol	Chain	Length	Quality of chain	
1	F	397	2%	70/ 60/
1	Г	521	87%	7% 6%
_	a	~~~	3%	
1	G	327	89%	6% 6%
			3%	
1	Н	327	87%	7% 6%
			9%	
1	Ι	327	83%	11% 6%
	_		6%	
1	J	327	84%	9% 6%
			2%	
1	K	327	85%	8% • 6%
	Ŧ		6%	
1	Ĺ	327	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
2	GLU	Κ	3360	-	Х	-	-
3	PEG	А	2002	-	-	Х	-
3	PEG	Κ	2001	-	-	Х	-



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.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
1	А	308	Total 2307	C 1456	N 395	O 450	S 6	0	1	0
1	В	308	Total 2310	C 1458	N 398	0 448	${f S}{6}$	0	1	0
1	Е	308	Total 2313	C 1461	N 396	0 450	S 6	0	2	0
1	F	308	Total 2307	C 1456	N 395	0 450	S 6	0	1	0
1	С	308	Total 2313	C 1461	N 396	0 450	${ m S}{ m 6}$	0	2	0
1	D	308	Total 2302	C 1453	N 395	O 448	${ m S}{ m 6}$	0	0	0
1	G	308	Total 2307	C 1456	N 395	O 450	${ m S}{ m 6}$	0	1	0
1	Н	308	Total 2315	C 1461	N 398	O 450	${ m S}{ m 6}$	0	2	0
1	Ι	308	Total 2302	C 1453	N 395	0 448	S 6	0	0	0
1	J	308	Total 2302	C 1453	N 395	0 448	${ m S}{ m 6}$	0	0	0
1	К	308	Total 2310	C 1458	N 398	0 448	${ m S}{ m 6}$	0	1	0
1	L	308	Total 2307	C 1456	N 395	0 450	$\begin{array}{c} \mathrm{S} \\ \mathrm{6} \end{array}$	0	1	0

• Molecule 1 is a protein called L-asparaginase.

• Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
0	٨	1	Total	С	Ν	0	0	0
	А	1	10	5	1	4	0	0
0	D	1	Total	С	Ν	0	0	0
	D	1	10	5	1	4	0	0
9	F	1	Total	С	Ν	0	0	0
	Ľ	1	10	5	1	4	0	0
9	F	1	Total	С	Ν	Ο	0	0
	Г	1	10	5	1	4	0	0
2	С	1	Total	С	Ν	0	0	0
	U	I	10	5	1	4	0	0
2	Л	1	Total	С	Ν	Ο	0	0
2	D	1	10	5	1	4	0	0
2	C	1	Total	С	Ν	Ο	0	0
2	ŭ	1	10	5	1	4	0	0
2	н	1	Total	С	Ν	Ο	0	0
2	11	1	10	5	1	4	0	0
2	Т	1	Total	С	Ν	Ο	0	0
2	I	1	10	5	1	4	0	0
2	Т	1	Total	С	Ν	Ο	0	0
2	0	T	10	5	1	4	0	0
2	K	1	Total	C	N	0	0	0
	17	1	10	5	1	4	0	0
2	T.	1	Total	C	N	0	0	0
		L	10	5	1	4		0

• Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
3	К	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	К	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	K	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
3	K	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	242	Total O 242 242	0	0
4	В	191	Total O 191 191	0	0
4	Ε	146	Total O 146 146	0	0
4	\mathbf{F}	241	Total O 241 241	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	229	Total O 229 229	0	0
4	D	109	Total O 109 109	0	0
4	G	145	Total O 145 145	0	0
4	Н	129	Total O 129 129	0	0
4	Ι	97	Total O 97 97	0	0
4	J	110	Total O 110 110	0	0
4	К	148	Total O 148 148	0	0
4	L	91	Total O 91 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.



• Molecule 1: L-asparaginase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	81.11Å 123.67Å 197.45Å	Deperitor
a, b, c, α , β , γ	90.00° 90.92° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	19.98 - 2.20	Depositor
Resolution (A)	19.98 - 2.20	EDS
% Data completeness	91.1 (19.98-2.20)	Depositor
(in resolution range)	91.1 (19.98-2.20)	EDS
R _{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.69 (at 2.19 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
B B.	0.220 , 0.267	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.217 , 0.262	DCC
R_{free} test set	9022 reflections (5.03%)	wwPDB-VP
Wilson B-factor $(Å^2)$	34.7	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.33 , 48.2	EDS
L-test for $twinning^2$	$< L >=0.51, < L^2>=0.35$	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.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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).

Mal	Chain	Bond	lengths	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.27	0/2344	0.50	0/3181
1	В	0.27	0/2347	0.50	0/3184
1	С	0.28	0/2353	0.50	0/3192
1	D	0.26	0/2336	0.47	0/3170
1	Е	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	Н	0.26	0/2355	0.48	0/3195
1	Ι	0.26	0/2336	0.48	0/3170
1	J	0.26	0/2336	0.48	0/3170
1	Κ	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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2307	0	2364	19	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	2310	0	2373	17	0
1	С	2313	0	2377	8	0
1	D	2302	0	2360	17	0
1	Е	2313	0	2377	18	0
1	F	2307	0	2364	15	0
1	G	2307	0	2364	11	0
1	Н	2315	0	2377	16	0
1	Ι	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	А	10	0	5	2	0
2	В	10	0	5	0	0
2	С	10	0	5	1	0
2	D	10	0	5	1	0
2	Е	10	0	5	1	0
2	F	10	0	5	1	0
2	G	10	0	5	0	0
2	Н	10	0	5	1	0
2	Ι	10	0	5	1	0
2	J	10	0	5	1	0
2	Κ	10	0	5	1	0
2	L	10	0	5	1	0
3	А	7	0	10	5	0
3	В	7	0	10	3	0
3	С	7	0	10	0	0
3	G	7	0	10	0	0
3	Κ	28	0	40	8	0
4	А	242	0	0	0	0
4	В	191	0	0	0	0
4	С	229	0	0	0	0
4	D	109	0	0	0	0
4	Е	146	0	0	0	0
4	F	241	0	0	0	0
4	G	145	0	0	0	0
4	Н	129	0	0	0	0
4	Ι	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	Clash
Atom-1	Atom-2	distance (Å)	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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		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	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: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
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: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



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		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
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: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:E:62:SER:OG	2:E:3352:GLU:O	2.25	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
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: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: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



2H	LN

		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
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: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: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



2H	LN

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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: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
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: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: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: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: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	А	305/327~(93%)	300 (98%)	4 (1%)	1 (0%)	41	46	
1	В	305/327~(93%)	297~(97%)	7 (2%)	1 (0%)	41	46	
1	С	306/327~(94%)	298 (97%)	7 (2%)	1 (0%)	41	46	
1	D	304/327~(93%)	296 (97%)	8 (3%)	0	100	100	
1	Е	306/327~(94%)	299 (98%)	7 (2%)	0	100	100	
1	F	305/327~(93%)	299 (98%)	5 (2%)	1 (0%)	41	46	
1	G	305/327~(93%)	296 (97%)	9 (3%)	0	100	100	
1	Н	306/327~(94%)	299~(98%)	7 (2%)	0	100	100	
1	Ι	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%)	41	46	
1	L	305/327~(93%)	296 (97%)	8 (3%)	1 (0%)	41	46	
All	All	3660/3924 (93%)	3565 (97%)	89 (2%)	6 (0%)	47	55	

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	204	THR
1	С	204	THR
1	А	204	THR
1	K	204	THR
1	В	204	THR
1	L	204	THR

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	252/261~(97%)	252 (100%)	0	100	100	
1	В	252/261~(97%)	248~(98%)	4 (2%)	62	76	
1	С	253/261~(97%)	253 (100%)	0	100	100	
1	D	251/261~(96%)	248~(99%)	3 (1%)	71	83	
1	Е	253/261~(97%)	252 (100%)	1 (0%)	91	96	
1	F	252/261~(97%)	252 (100%)	0	100	100	
1	G	252/261~(97%)	252 (100%)	0	100	100	
1	Н	253/261~(97%)	252 (100%)	1 (0%)	91	96	
1	Ι	251/261~(96%)	250 (100%)	1 (0%)	91	96	
1	J	251/261~(96%)	250 (100%)	1 (0%)	91	96	
1	Κ	252/261~(97%)	250 (99%)	2 (1%)	81	90	
1	L	252/261~(97%)	251 (100%)	1 (0%)	91	96	
All	All	3024/3132~(97%)	3010 (100%)	14 (0%)	88	94	

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

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	76	ARG
1	В	206[A]	ARG
1	В	206[B]	ARG
1	В	239	LYS
1	Е	321	GLN
1	D	99	ASP
1	D	178	LYS
1	D	258	ARG
1	Н	3	ASN
1	Ι	145	LYS
1	J	3	ASN
1	K	145	LYS
1	К	257	LYS
1	L	321	GLN

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



Mol	Chain	Res	Type
1	А	196	GLN
1	В	3	ASN
1	Е	146	ASN
1	Е	325	HIS
1	F	196	GLN
1	С	3	ASN
1	С	41	GLN
1	D	290	GLN
1	D	325	HIS
1	G	146	ASN
1	G	196	GLN
1	Н	3	ASN
1	Ι	3	ASN
1	Ι	196	GLN
1	Ι	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 (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 monosaccharides 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	Tuno	Chain	Dog	Link	B	ond leng	gths	Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	В	2003	-	6,6,6	0.52	0	$5,\!5,\!5$	0.21	0
2	GLU	L	3361	-	8,9,9	1.01	1 (12%)	10,11,11	1.38	2 (20%)
2	GLU	Ι	3358	-	8,9,9	1.03	1 (12%)	10,11,11	1.41	2 (20%)
2	GLU	K	3360	-	8,9,9	1.02	1 (12%)	10,11,11	1.42	2 (20%)
3	PEG	К	2001	-	6,6,6	0.51	0	$5,\!5,\!5$	0.17	0
2	GLU	А	3350	-	8,9,9	1.01	1 (12%)	10,11,11	1.35	2 (20%)
3	PEG	С	2004	-	6,6,6	0.44	0	$5,\!5,\!5$	0.29	0
2	GLU	J	3351	-	8,9,9	1.02	1 (12%)	10,11,11	1.38	2 (20%)
2	GLU	Н	3357	-	8,9,9	1.01	1 (12%)	10,11,11	1.42	2 (20%)
3	PEG	K	2007	-	6,6,6	0.45	0	$5,\!5,\!5$	0.30	0
2	GLU	В	3359	-	8,9,9	1.06	1 (12%)	10,11,11	1.35	2 (20%)
2	GLU	D	3355	-	8,9,9	1.02	1 (12%)	10,11,11	1.41	2 (20%)
3	PEG	K	2008	-	6,6,6	0.46	0	$5,\!5,\!5$	0.25	0
2	GLU	Е	3352	-	8,9,9	1.03	1 (12%)	10,11,11	1.38	2 (20%)
3	PEG	K	2005	-	6,6,6	0.45	0	$5,\!5,\!5$	0.30	0
2	GLU	G	3356	-	8,9,9	1.04	1 (12%)	10,11,11	1.40	2 (20%)
2	GLU	F	3353	-	8,9,9	1.04	1 (12%)	10,11,11	1.36	2 (20%)
3	PEG	G	2006	-	$6,\!6,\!6$	0.45	0	$5,\!5,\!5$	0.26	0
3	PEG	A	2002	_	6,6,6	0.47	0	$5,\!5,\!5$	0.18	0
2	GLU	С	3354	-	8,9,9	1.03	1 (12%)	10,11,11	1.38	2 (20%)

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	В	2003	-	-	2/4/4/4	-
2	GLU	L	3361	-	-	8/9/9/9	-
2	GLU	Ι	3358	-	-	5/9/9/9	-
2	GLU	K	3360	-	-	9/9/9/9	-
3	PEG	К	2001	-	-	1/4/4/4	-
2	GLU	А	3350	-	-	3/9/9/9	-
3	PEG	С	2004	-	-	4/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	J	3351	-	-	5/9/9/9	-
2	GLU	Н	3357	-	-	5/9/9/9	-
3	PEG	K	2007	-	-	3/4/4/4	-
2	GLU	В	3359	-	-	5/9/9/9	-
2	GLU	D	3355	-	-	5/9/9/9	-
3	PEG	K	2008	-	-	1/4/4/4	-
2	GLU	Е	3352	-	-	5/9/9/9	-
3	PEG	Κ	2005	-	-	3/4/4/4	-
2	GLU	G	3356	-	-	5/9/9/9	-
2	GLU	F	3353	-	-	5/9/9/9	-
3	PEG	G	2006	-	-	3/4/4/4	-
3	PEG	А	2002	-	-	4/4/4/4	-
2	GLU	С	3354	-	-	5/9/9/9	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	3359	GLU	OXT-C	-2.25	1.23	1.30
2	С	3354	GLU	OXT-C	-2.20	1.23	1.30
2	G	3356	GLU	OXT-C	-2.17	1.23	1.30
2	D	3355	GLU	OXT-C	-2.15	1.23	1.30
2	J	3351	GLU	OXT-C	-2.14	1.23	1.30
2	Ε	3352	GLU	OXT-C	-2.13	1.23	1.30
2	Κ	3360	GLU	OXT-C	-2.12	1.23	1.30
2	F	3353	GLU	OXT-C	-2.11	1.23	1.30
2	Н	3357	GLU	OXT-C	-2.11	1.23	1.30
2	Ι	3358	GLU	OXT-C	-2.09	1.23	1.30
2	Ĺ	3361	GLU	OXT-C	-2.08	1.23	1.30
2	А	3350	GLU	OXT-C	-2.06	1.23	1.30

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	D	3355	GLU	OXT-C-O	-2.85	117.63	124.09
2	Κ	3360	GLU	OXT-C-O	-2.84	117.64	124.09
2	Ι	3358	GLU	OXT-C-O	-2.77	117.79	124.09
2	Н	3357	GLU	OXT-C-O	-2.75	117.85	124.09
2	G	3356	GLU	OXT-C-O	-2.75	117.86	124.09
2	В	3359	GLU	OXT-C-O	-2.72	117.92	124.09



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	3354	GLU	OXT-C-O	-2.72	117.92	124.09
2	Ε	3352	GLU	OXT-C-O	-2.68	118.01	124.09
2	F	3353	GLU	OXT-C-O	-2.66	118.06	124.09
2	J	3351	GLU	OXT-C-O	-2.65	118.08	124.09
2	А	3350	GLU	OXT-C-O	-2.64	118.09	124.09
2	L	3361	GLU	OXT-C-O	-2.63	118.12	124.09
2	Κ	3360	GLU	OXT-C-CA	2.39	121.51	113.38
2	D	3355	GLU	OXT-C-CA	2.34	121.35	113.38
2	G	3356	GLU	OXT-C-CA	2.32	121.28	113.38
2	Ι	3358	GLU	OXT-C-CA	2.31	121.25	113.38
2	А	3350	GLU	OXT-C-CA	2.31	121.25	113.38
2	Е	3352	GLU	OXT-C-CA	2.29	121.19	113.38
2	С	3354	GLU	OXT-C-CA	2.29	121.19	113.38
2	J	3351	GLU	OXT-C-CA	2.29	121.17	113.38
2	L	3361	GLU	OXT-C-CA	2.28	121.16	113.38
2	Н	3357	GLU	OXT-C-CA	2.27	121.13	113.38
2	В	3359	GLU	OXT-C-CA	2.24	121.02	113.38
2	F	3353	GLU	OXT-C-CA	2.23	120.99	113.38

There are no chirality outliers.

All (86) torsion outliers are listed be	rsion outliers are listed be	low:
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Mol	Chain	\mathbf{Res}	Type	Atoms
2	L	3361	GLU	O-C-CA-N
2	Κ	3360	GLU	OXT-C-CA-N
2	D	3355	GLU	OXT-C-CA-N
2	G	3356	GLU	OXT-C-CA-N
2	L	3361	GLU	OXT-C-CA-N
3	В	2003	PEG	O1-C1-C2-O2
3	С	2004	PEG	O1-C1-C2-O2
3	А	2002	PEG	O1-C1-C2-O2
3	Κ	2001	PEG	O2-C3-C4-O4
3	Κ	2005	PEG	O2-C3-C4-O4
2	В	3359	GLU	OXT-C-CA-N
3	А	2002	PEG	O2-C3-C4-O4
2	L	3361	GLU	CA-CB-CG-CD
2	F	3353	GLU	OXT-C-CA-N
2	С	3354	GLU	OXT-C-CA-N
2	Ι	3358	GLU	CA-CB-CG-CD
3	Κ	2008	PEG	C1-C2-O2-C3
2	А	3350	GLU	OXT-C-CA-N
2	Е	3352	GLU	CA-CB-CG-CD



Mol	Chain	Res	Type	Atoms
2	Е	3352	GLU	OXT-C-CA-N
2	Ι	3358	GLU	OXT-C-CA-N
3	С	2004	PEG	O2-C3-C4-O4
3	K	2007	PEG	O1-C1-C2-O2
2	J	3351	GLU	OXT-C-CA-N
3	G	2006	PEG	O2-C3-C4-O4
2	А	3350	GLU	O-C-CA-N
2	В	3359	GLU	O-C-CA-N
2	Е	3352	GLU	O-C-CA-N
2	F	3353	GLU	O-C-CA-N
2	С	3354	GLU	O-C-CA-N
2	D	3355	GLU	O-C-CA-N
2	G	3356	GLU	O-C-CA-N
2	Ι	3358	GLU	O-C-CA-N
2	J	3351	GLU	O-C-CA-N
2	K	3360	GLU	O-C-CA-N
3	K	2007	PEG	C4-C3-O2-C2
3	С	2004	PEG	C4-C3-O2-C2
3	G	2006	PEG	C4-C3-O2-C2
3	K	2005	PEG	C4-C3-O2-C2
3	А	2002	PEG	C1-C2-O2-C3
2	В	3359	GLU	CA-CB-CG-CD
2	Н	3357	GLU	CA-CB-CG-CD
3	K	2007	PEG	C1-C2-O2-C3
2	Н	3357	GLU	OXT-C-CA-N
3	G	2006	PEG	O1-C1-C2-O2
2	K	3360	GLU	N-CA-CB-CG
2	L	3361	GLU	N-CA-CB-CG
3	С	2004	PEG	C1-C2-O2-C3
2	L	3361	GLU	OXT-C-CA-CB
2	С	3354	GLU	CA-CB-CG-CD
3	A	2002	PEG	C4-C3-O2-C2
2	G	3356	GLU	CA-CB-CG-CD
2	K	3360	GLU	CA-CB-CG-CD
3	В	2003	PEG	C1-C2-O2-C3
2	L	3361	GLU	O-C-CA-CB
2	G	3356	GLU	OE1-CD-CG-CB
2	L	3361	GLU	OE1-CD-CG-CB
2	J	3351	GLU	OE2-CD-CG-CB
2	D	3355	GLU	CA-CB-CG-CD
2	G	3356	GLU	OE2-CD-CG-CB
2	J	3351	GLU	OE1-CD-CG-CB



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Mol	Chain	Res	Type	Atoms
2	L	3361	GLU	OE2-CD-CG-CB
2	Κ	3360	GLU	OE2-CD-CG-CB
2	Н	3357	GLU	O-C-CA-N
2	K	3360	GLU	OE1-CD-CG-CB
2	С	3354	GLU	OE2-CD-CG-CB
2	F	3353	GLU	OE2-CD-CG-CB
2	Е	3352	GLU	OE2-CD-CG-CB
2	Н	3357	GLU	OE2-CD-CG-CB
2	В	3359	GLU	OE2-CD-CG-CB
2	D	3355	GLU	OE2-CD-CG-CB
2	D	3355	GLU	OE1-CD-CG-CB
2	С	3354	GLU	OE1-CD-CG-CB
2	Н	3357	GLU	OE1-CD-CG-CB
2	Ι	3358	GLU	OE1-CD-CG-CB
2	Ι	3358	GLU	OE2-CD-CG-CB
2	K	3360	GLU	C-CA-CB-CG
2	Е	3352	GLU	OE1-CD-CG-CB
2	А	3350	GLU	CA-CB-CG-CD
2	J	3351	GLU	CA-CB-CG-CD
2	В	3359	GLU	OE1-CD-CG-CB
2	F	3353	GLU	OE1-CD-CG-CB
2	F	3353	GLU	CA-CB-CG-CD
2	K	3360	GLU	OXT-C-CA-CB
2	К	3360	GLU	O-C-CA-CB
3	K	2005	PEG	O1-C1-C2-O2

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There are no ring outliers.

15 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	2003	PEG	3	0
2	L	3361	GLU	1	0
2	Ι	3358	GLU	1	0
2	Κ	3360	GLU	1	0
3	Κ	2001	PEG	5	0
2	А	3350	GLU	2	0
2	J	3351	GLU	1	0
2	Н	3357	GLU	1	0
3	Κ	2007	PEG	1	0
2	D	3355	GLU	1	0
3	K	2008	PEG	2	0
2	Е	3352	GLU	1	0



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Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
2	F	3353	GLU	1	0
3	А	2002	PEG	5	0
2	С	3354	GLU	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	А	308/327~(94%)	-0.40	8 (2%) 56 53	17, 28, 47, 126	0
1	В	308/327~(94%)	-0.28	8 (2%) 56 53	19, 33, 61, 105	0
1	С	308/327~(94%)	-0.39	5 (1%) 72 70	19, 30, 51, 91	0
1	D	308/327~(94%)	0.16	13 (4%) 36 34	26, 48, 76, 150	0
1	E	308/327~(94%)	0.10	14 (4%) 33 32	22, 41, 72, 143	0
1	F	308/327~(94%)	-0.43	7 (2%) 60 58	17, 28, 53, 106	0
1	G	308/327~(94%)	-0.13	11 (3%) 42 41	18, 38, 70, 124	0
1	Н	308/327~(94%)	-0.04	9 (2%) 51 49	26, 42, 70, 128	0
1	Ι	308/327~(94%)	0.52	31 (10%) 7 6	24, 50, 103, 147	0
1	J	308/327~(94%)	0.24	20 (6%) 18 17	28, 48, 85, 152	0
1	K	308/327~(94%)	-0.19	7 (2%) 60 58	22, 35, 73, 114	0
1	L	308/327~(94%)	0.39	18 (5%) 23 22	28, 50, 80, 147	0
All	All	3696/3924 (94%)	-0.04	151 (4%) 37 35	17, 39, 78, 152	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	35	GLY	12.6
1	Ι	35	GLY	11.0
1	Е	35	GLY	10.3
1	J	36	VAL	7.8
1	D	36	VAL	7.2
1	Ι	36	VAL	6.9
1	L	16	ILE	6.8
1	J	35	GLY	6.3
1	D	39	LEU	5.9
1	J	39	LEU	5.8
1	L	35	GLY	5.8



Mol	Chain	Res	Type	RSRZ
1	Е	17	ALA	5.5
1	K	3	ASN	5.5
1	L	3	ASN	5.3
1	D	288	ALA	5.2
1	Ι	213	ASN	5.2
1	Е	36	VAL	5.1
1	L	15	THR	5.0
1	Ι	17	ALA	4.8
1	Ι	47	LYS	4.8
1	А	35	GLY	4.8
1	Ι	84	SER	4.7
1	В	35	GLY	4.7
1	С	39	LEU	4.6
1	J	125	THR	4.5
1	D	3	ASN	4.5
1	А	38	THR	4.4
1	F	36	VAL	4.2
1	Н	39	LEU	4.1
1	L	36	VAL	4.1
1	Ι	38	THR	4.1
1	J	15	THR	4.0
1	Е	41	GLN	4.0
1	Н	41	GLN	3.9
1	L	205	THR	3.8
1	Ι	3	ASN	3.8
1	D	110	LYS	3.8
1	Ι	215	ASP	3.7
1	В	3	ASN	3.6
1	Ι	125	THR	3.6
1	J	38	THR	3.5
1	A	39	LEU	3.4
1	J	16	ILE	3.4
1	A	36	VAL	3.4
1	I	48	THR	3.4
1	G	3	ASN	3.4
1	J	213	ASN	3.4
1	Н	35	GLY	3.3
1	С	36	VAL	3.3
1	G	125	THR	3.3
1	Ι	90	VAL	3.2
1	J	59	SER	3.2
1	L	17	ALA	3.2



Mol	Chain	Res	Type	RSRZ
1	Ι	82	ALA	3.2
1	Е	3	ASN	3.1
1	J	54	GLY	3.1
1	L	213	ASN	3.1
1	G	39	LEU	3.1
1	Н	4	LEU	3.1
1	Н	59	SER	3.1
1	А	40	ILE	3.1
1	Ι	216	LYS	3.0
1	L	318	ALA	3.0
1	D	206	ARG	3.0
1	Ι	51	ASN	3.0
1	G	41	GLN	3.0
1	L	41	GLN	2.9
1	С	35	GLY	2.9
1	K	36	VAL	2.9
1	Н	15	THR	2.9
1	L	90	VAL	2.9
1	G	17	ALA	2.9
1	Ι	15	THR	2.9
1	Ι	145	LYS	2.9
1	D	213	ASN	2.8
1	Ι	79	GLU	2.8
1	Н	17	ALA	2.8
1	F	15	THR	2.8
1	F	3	ASN	2.8
1	Е	54	GLY	2.7
1	D	289	GLY	2.7
1	Ι	214	VAL	2.7
1	K	125	THR	2.7
1	Е	213	ASN	2.7
1	Ι	4	LEU	2.7
1	С	3	ASN	2.7
1	J	3	ASN	2.7
1	Е	60	ILE	2.6
1	L	125	THR	2.6
1	L	145	LYS	2.6
1	G	38	THR	2.6
1	С	38	THR	2.5
1	В	39	LEU	2.5
1	К	49	LEU	2.5
1	G	35	GLY	2.5



Mol	Chain	Res	Type	RSRZ
1	J	47	LYS	2.5
1	Е	38	THR	2.5
1	В	17	ALA	2.5
1	Ι	6	ASN	2.5
1	Ι	83	ARG	2.4
1	F	125	THR	2.4
1	Ι	16	ILE	2.4
1	Ι	37	GLU	2.4
1	L	212	THR	2.4
1	Е	105	LEU	2.4
1	G	42	ALA	2.4
1	Ι	44	PRO	2.4
1	Ι	52	ILE	2.4
1	K	41	GLN	2.3
1	А	15	THR	2.3
1	J	212	THR	2.3
1	Ι	60	ILE	2.3
1	F	17	ALA	2.3
1	Н	60	ILE	2.3
1	Ι	56	GLN	2.3
1	F	44	PRO	2.3
1	В	56	GLN	2.3
1	J	289	GLY	2.3
1	Ι	211	VAL	2.3
1	J	315	THR	2.2
1	G	145	LYS	2.2
1	Ι	41	GLN	2.2
1	Ι	8	VAL	2.2
1	J	40	ILE	2.2
1	В	38	THR	2.2
1	Е	314	THR	2.2
1	D	15	THR	2.2
1	Н	91	ILE	2.2
1	F	35	GLY	2.2
1	Е	15	THR	2.1
1	L	38	THR	2.1
1	J	17	ALA	2.1
1	L	4	LEU	2.1
1	K	48	THR	2.1
1	J	41	GLN	2.1
1	В	37	GLU	2.1
1	Е	40	ILE	2.1



Mol	Chain	Res	Type	RSRZ
1	D	16	ILE	2.1
1	G	59	SER	2.1
1	В	41	GLN	2.1
1	L	261	ALA	2.1
1	А	257	LYS	2.1
1	D	205	THR	2.1
1	А	288	ALA	2.1
1	Ε	37	GLU	2.0
1	D	112	ASP	2.0
1	G	53	LYS	2.0
1	J	215	ASP	2.0
1	Κ	39	LEU	2.0
1	L	127	ILE	2.0
1	J	83	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
3	PEG	K	2008	7/7	0.69	0.25	59,64,71,73	0
3	PEG	G	2006	7/7	0.74	0.22	$36{,}53{,}65{,}68$	0
3	PEG	K	2005	7/7	0.77	0.26	58,66,70,72	0
3	PEG	K	2007	7/7	0.78	0.25	59,73,81,83	0
3	PEG	K	2001	7/7	0.79	0.22	16,26,47,57	0
2	GLU	L	3361	10/10	0.82	0.18	40,50,62,70	0
2	GLU	J	3351	10/10	0.82	0.18	59,63,69,70	0
3	PEG	С	2004	7/7	0.83	0.21	43,64,78,82	0
3	PEG	А	2002	7/7	0.87	0.21	$19,\!38,\!50,\!59$	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
3	PEG	В	2003	7/7	0.88	0.20	10,24,48,58	0
2	GLU	Н	3357	10/10	0.90	0.17	46,52,61,75	0
2	GLU	Ι	3358	10/10	0.90	0.12	38,44,54,56	0
2	GLU	Е	3352	10/10	0.90	0.13	$36,\!44,\!55,\!59$	0
2	GLU	F	3353	10/10	0.94	0.12	24,38,43,45	0
2	GLU	D	3355	10/10	0.94	0.11	$40,\!43,\!57,\!57$	0
2	GLU	K	3360	10/10	0.95	0.09	$29,\!37,\!53,\!57$	0
2	GLU	В	3359	10/10	0.95	0.10	27,28,49,52	0
2	GLU	А	3350	10/10	0.96	0.10	23,32,39,40	0
2	GLU	C	3354	10/10	0.96	0.09	28,34,39,52	0
2	GLU	G	3356	10/10	0.97	0.10	33,41,50,60	0

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6.5 Other polymers (i)

There are no such residues in this entry.

