



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 10:09 pm BST

PDB ID : 4JEQ
Title : Different Contribution of Conserved Amino Acids to the Global Properties of Homologous Enzymes
Authors : Hernandez-Santoyo, A.; Aguirre-Fuentes, Y.; Torres-Larios, A.; Gomez-Puyou, A.; De Gomez-Puyou, M.T.
Deposited on : 2013-02-27
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

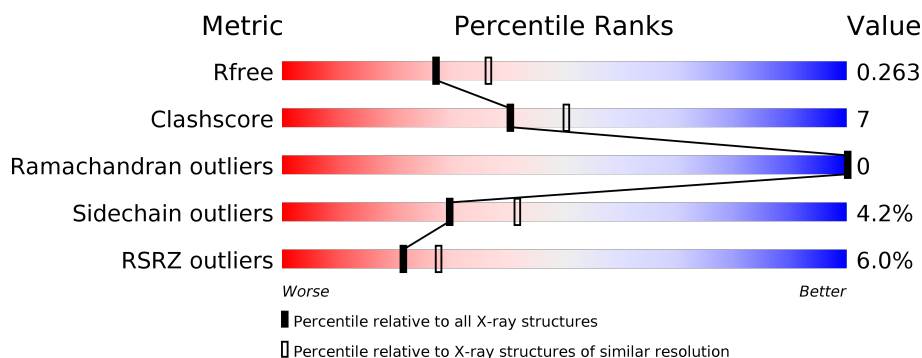
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	250	
1	B	250	
1	C	250	
1	D	250	
1	E	250	
1	F	250	

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Mol	Chain	Length	Quality of chain
1	G	250	
1	H	250	
1	I	250	
1	J	250	
1	K	250	
1	L	250	

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	B	301	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23118 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 TRIOSEPHOSPHATE ISOMERASE, GLYCOSOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1890	1201	332	351	6			
1	B	245	Total	C	N	O	S	0	0	0
			1858	1182	326	344	6			
1	C	248	Total	C	N	O	S	0	0	0
			1879	1195	330	348	6			
1	D	250	Total	C	N	O	S	0	0	0
			1889	1201	332	350	6			
1	E	250	Total	C	N	O	S	0	0	0
			1885	1197	331	351	6			
1	F	249	Total	C	N	O	S	0	0	0
			1883	1197	331	349	6			
1	G	245	Total	C	N	O	S	0	0	0
			1856	1179	326	345	6			
1	H	243	Total	C	N	O	S	0	0	0
			1841	1171	324	341	5			
1	I	247	Total	C	N	O	S	0	0	0
			1870	1189	329	346	6			
1	J	249	Total	C	N	O	S	0	0	0
			1882	1197	331	348	6			
1	K	246	Total	C	N	O	S	0	0	0
			1865	1187	327	345	6			
1	L	246	Total	C	N	O	S	0	0	0
			1866	1187	328	345	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	ASP	GLU	ENGINEERED MUTATION	UNP P04789
B	104	ASP	GLU	ENGINEERED MUTATION	UNP P04789
C	104	ASP	GLU	ENGINEERED MUTATION	UNP P04789
D	104	ASP	GLU	ENGINEERED MUTATION	UNP P04789
E	104	ASP	GLU	ENGINEERED MUTATION	UNP P04789

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Chain	Residue	Modelled	Actual	Comment	Reference
F	104	ASP	GLU	ENGINEERED MUTATION	UNP P04789
G	104	ASP	GLU	ENGINEERED MUTATION	UNP P04789
H	104	ASP	GLU	ENGINEERED MUTATION	UNP P04789
I	104	ASP	GLU	ENGINEERED MUTATION	UNP P04789
J	104	ASP	GLU	ENGINEERED MUTATION	UNP P04789
K	104	ASP	GLU	ENGINEERED MUTATION	UNP P04789
L	104	ASP	GLU	ENGINEERED MUTATION	UNP P04789

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		
4	B	85	Total	O	0	0
			85	85		
4	C	65	Total	O	0	0
			65	65		
4	D	84	Total	O	0	0
			84	84		
4	E	72	Total	O	0	0
			72	72		
4	F	43	Total	O	0	0
			43	43		
4	G	27	Total	O	0	0
			27	27		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	22	Total 22	O 22	0	0
4	I	18	Total 18	O 18	0	0
4	J	12	Total 12	O 12	0	0
4	K	14	Total 14	O 14	0	0
4	L	13	Total 13	O 13	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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.

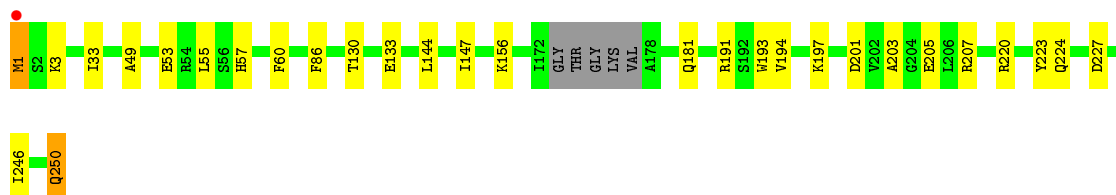
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE, GLYCOSOMAL

Chain A: 




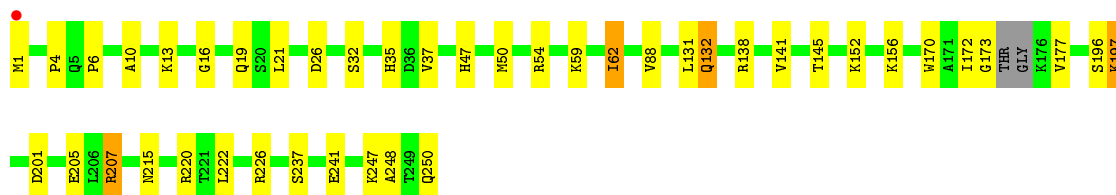
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Chain B: 

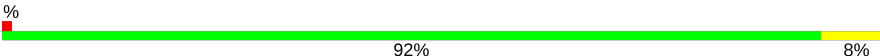


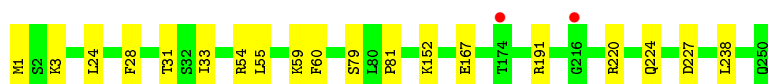
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE, GLYCOSOMAL

Chain C: 



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE, GLYCOSOMAL

Chain D: 

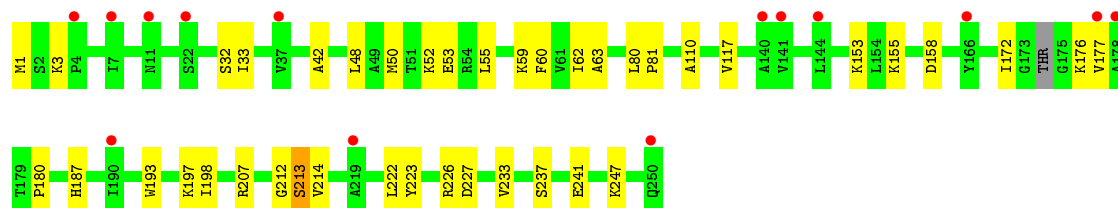
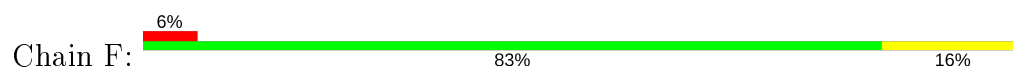


• Molecule 1: TRIOSEPHOSPHATE ISOMERASE, GLYCOSOMAL

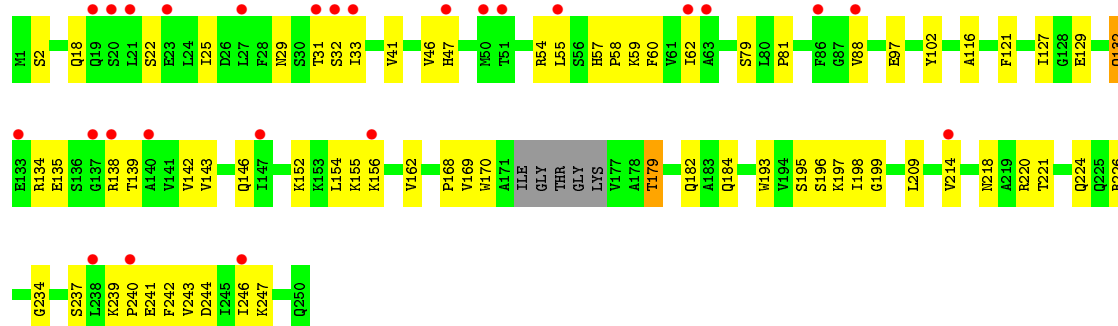
Chain E: 



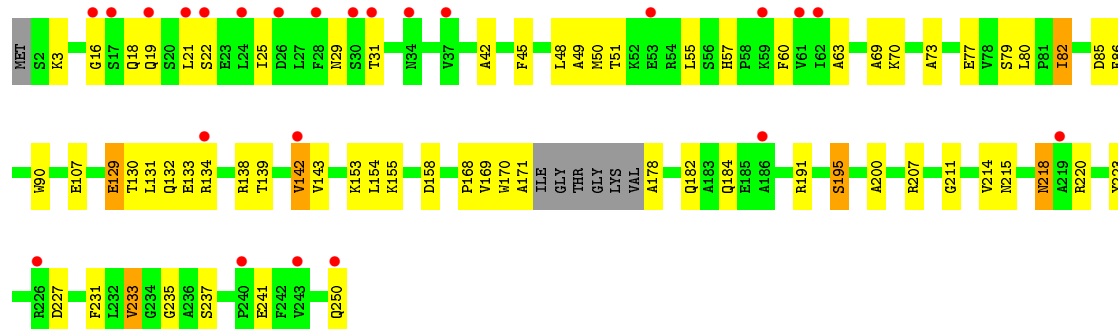
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE, GLYCOSOMAL



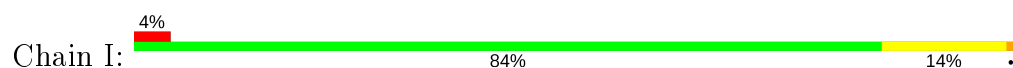
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE, GLYCOSOMAL

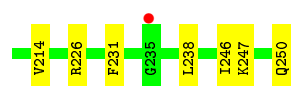


- Molecule 1: TRIOSEPHOSPHATE ISOMERASE, GLYCOSOMAL

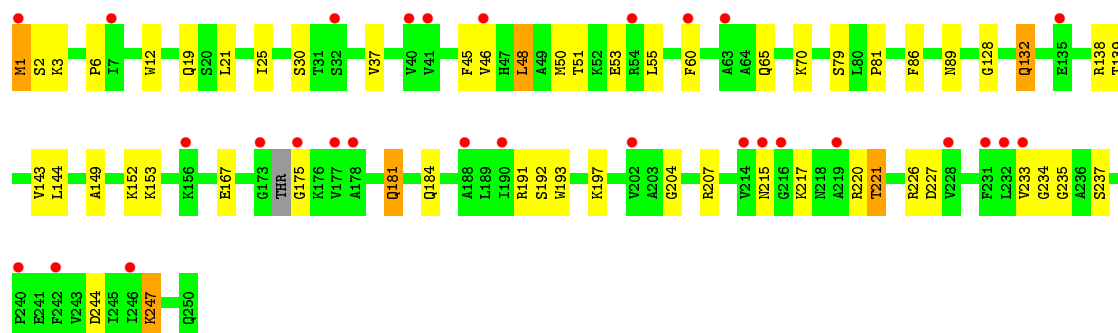
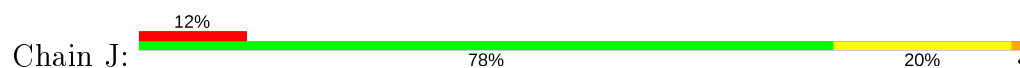


- Molecule 1: TRIOSEPHOSPHATE ISOMERASE, GLYCOSOMAL

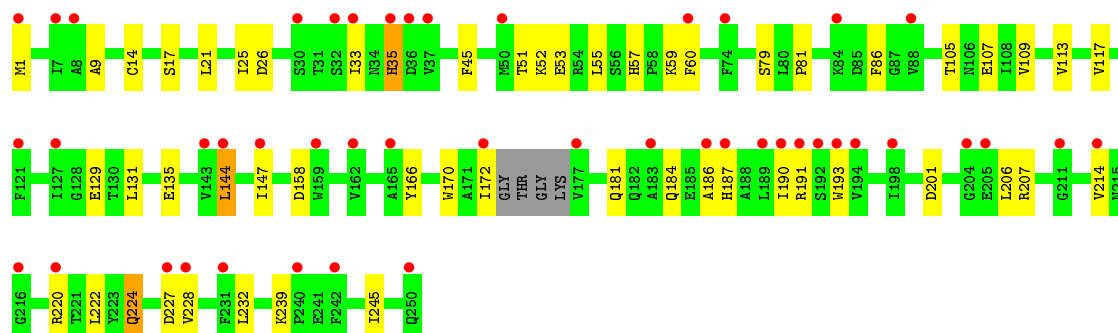
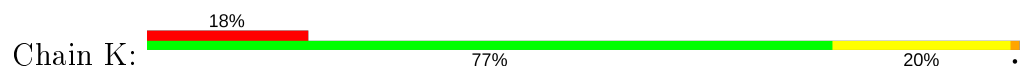




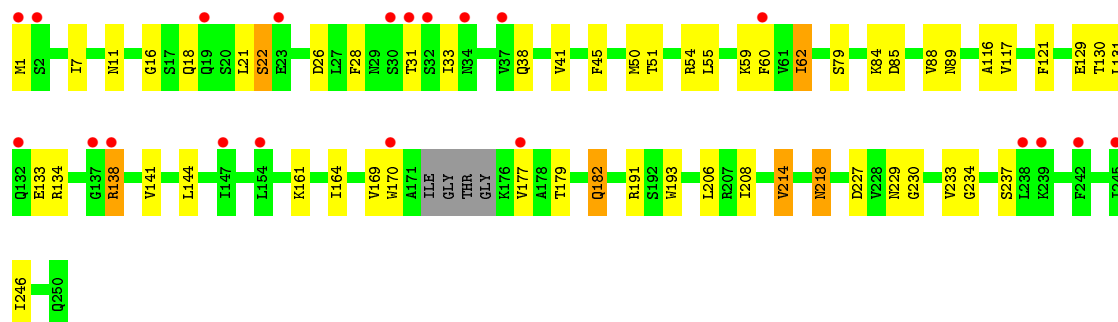
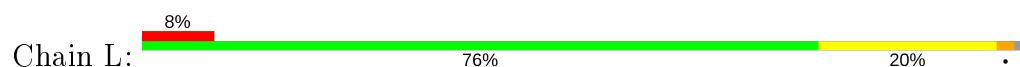
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE, GLYCOSOMAL



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE, GLYCOSOMAL



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE, GLYCOSOMAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.09Å 89.78Å 181.72Å 90.00° 101.61° 90.00°	Depositor
Resolution (Å)	61.58 – 2.30 89.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (61.58-2.30) 95.6 (89.00-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1307)	Depositor
R, R_{free}	0.207 , 0.261 0.208 , 0.263	Depositor DCC
R_{free} test set	6152 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23118	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% 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, SO4

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	0.49	0/1924	0.61	0/2608
1	B	0.48	0/1891	0.60	0/2564
1	C	0.44	0/1912	0.57	0/2590
1	D	0.49	0/1923	0.56	0/2608
1	E	0.53	1/1919 (0.1%)	0.61	1/2602 (0.0%)
1	F	0.46	0/1916	0.55	0/2595
1	G	0.42	0/1889	0.56	0/2560
1	H	0.47	0/1874	0.55	0/2542
1	I	0.48	0/1903	0.54	0/2579
1	J	0.39	0/1915	0.54	0/2595
1	K	0.34	0/1898	0.49	0/2574
1	L	0.36	0/1899	0.51	0/2574
All	All	0.45	1/22863 (0.0%)	0.56	1/30991 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	170	TRP	NE1-CE2	-5.25	1.30	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	173	GLY	N-CA-C	-5.15	100.23	113.10

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	1890	0	1927	14	0
1	B	1858	0	1891	26	0
1	C	1879	0	1916	27	0
1	D	1889	0	1927	9	0
1	E	1885	0	1915	12	0
1	F	1883	0	1919	20	0
1	G	1856	0	1882	53	0
1	H	1841	0	1865	53	0
1	I	1870	0	1905	33	0
1	J	1882	0	1919	35	0
1	K	1865	0	1900	32	0
1	L	1866	0	1902	34	0
2	A	5	0	0	0	0
2	D	10	0	0	0	0
2	H	5	0	0	1	0
2	K	5	0	0	0	0
3	A	7	0	10	3	0
3	B	14	0	20	6	0
3	C	7	0	9	3	0
3	E	7	0	9	0	0
4	A	139	0	0	2	0
4	B	85	0	0	0	0
4	C	65	0	0	3	0
4	D	84	0	0	1	0
4	E	72	0	0	0	0
4	F	43	0	0	1	0
4	G	27	0	0	3	0
4	H	22	0	0	1	0
4	I	18	0	0	0	0
4	J	12	0	0	1	0
4	K	14	0	0	2	0
4	L	13	0	0	0	0
All	All	23118	0	22916	326	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 7.

All (326) 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:205:GLU:CG	1:I:1:MET:HB3	1.70	1.20
1:J:234:GLY:O	1:J:237:SER:HB3	1.43	1.17
1:B:205:GLU:HG2	1:I:1:MET:HB3	1.16	1.12
1:B:205:GLU:HG2	1:I:1:MET:CB	1.86	1.05
1:C:6:PRO:HG2	1:C:37:VAL:HG22	1.45	0.96
1:G:179:THR:H	1:G:182:GLN:HE21	1.08	0.95
1:A:57:HIS:HD2	1:A:59:LYS:H	1.14	0.94
1:K:57:HIS:HD2	1:K:59:LYS:H	1.16	0.94
1:H:170:TRP:O	1:H:170:TRP:CD1	2.29	0.84
1:G:134:ARG:HH21	1:G:139:THR:HG21	1.41	0.81
1:H:25:ILE:HD11	1:H:51:THR:HG22	1.66	0.78
1:B:3:LYS:HD2	3:B:302:PEG:H41	1.69	0.75
1:H:233:VAL:HG22	1:H:237:SER:HB3	1.69	0.73
1:L:208:ILE:H	1:L:229:ASN:HD22	1.36	0.72
1:B:86:PHE:CZ	3:B:301:PEG:H31	2.24	0.72
1:K:224:GLN:NE2	4:K:402:HOH:O	2.24	0.71
1:H:220:ARG:NH1	1:H:250:GLN:O	2.23	0.70
1:J:25:ILE:HD11	1:J:51:THR:HG22	1.74	0.70
1:F:3:LYS:NZ	1:F:223:TYR:O	2.24	0.69
1:J:6:PRO:HG2	1:J:37:VAL:HG22	1.75	0.68
1:K:35:HIS:O	1:K:59:LYS:NZ	2.26	0.68
1:H:170:TRP:HD1	1:H:170:TRP:O	1.74	0.68
1:I:3:LYS:HE3	1:I:226:ARG:O	1.94	0.67
1:C:13:LYS:NZ	3:C:301:PEG:H31	2.10	0.67
1:H:168:PRO:HD2	1:H:211:GLY:O	1.96	0.66
1:L:191:ARG:HH22	1:L:229:ASN:HD21	1.42	0.66
1:K:144:LEU:HG	1:K:193:TRP:CD1	2.31	0.65
1:I:25:ILE:HD11	1:I:51:THR:HG22	1.77	0.65
1:J:152:LYS:HE2	1:J:153:LYS:HZ3	1.61	0.65
1:L:131:LEU:HA	1:L:170:TRP:HB3	1.79	0.65
1:C:35:HIS:O	1:C:59:LYS:NZ	2.25	0.64
1:G:32:SER:O	1:G:247:LYS:NZ	2.30	0.64
1:A:20:SER:HB2	3:A:302:PEG:H21	1.78	0.64
1:B:53:GLU:HB2	3:B:301:PEG:H11	1.79	0.64
1:K:9:ALA:HB3	1:K:232:LEU:HA	1.80	0.64
1:G:129:GLU:OE2	1:G:170:TRP:NE1	2.30	0.63
1:J:12:TRP:HD1	1:J:237:SER:HG	1.46	0.63
1:D:33:ILE:O	1:D:59:LYS:NZ	2.31	0.62
1:F:1:MET:HG2	1:F:226:ARG:HG3	1.81	0.62
1:A:225:GLN:NE2	4:A:438:HOH:O	2.33	0.62
1:J:233:VAL:HG13	1:J:237:SER:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:129:GLU:O	1:H:169:VAL:HG23	1.99	0.61
1:L:214:VAL:HA	1:L:218:ASN:HD21	1.65	0.61
1:H:169:VAL:O	1:H:171:ALA:N	2.29	0.61
1:L:55:LEU:HD21	1:L:60:PHE:HB3	1.83	0.61
1:G:46:VAL:HG21	1:H:82:ILE:HD11	1.83	0.60
1:J:152:LYS:HG3	1:J:153:LYS:HZ3	1.66	0.60
1:H:55:LEU:HD11	1:H:60:PHE:HB2	1.82	0.60
1:G:62:ILE:HD13	1:G:88:VAL:HG22	1.83	0.60
1:G:152:LYS:HB2	4:G:318:HOH:O	2.02	0.60
1:K:57:HIS:CD2	1:K:59:LYS:H	2.07	0.60
1:I:247:LYS:NZ	1:K:17:SER:OG	2.35	0.59
1:C:13:LYS:HZ1	3:C:301:PEG:H31	1.67	0.59
1:G:179:THR:H	1:G:182:GLN:NE2	1.89	0.59
1:J:79:SER:HB2	1:J:81:PRO:HD2	1.86	0.58
1:J:175:GLY:N	4:J:312:HOH:O	2.37	0.57
1:A:10:ALA:HB1	1:A:237:SER:HB2	1.86	0.57
1:A:57:HIS:CD2	1:A:59:LYS:H	2.07	0.57
1:H:107:GLU:OE2	1:H:153:LYS:NZ	2.37	0.57
1:C:16:GLY:HA3	1:C:21:LEU:HD11	1.86	0.57
1:E:127:ILE:HD12	1:E:143:VAL:HG13	1.86	0.57
1:H:130:THR:HA	1:H:169:VAL:HB	1.85	0.57
1:L:11:ASN:O	1:L:234:GLY:HA2	2.05	0.57
1:J:139:THR:O	1:J:143:VAL:HG12	2.05	0.56
1:G:18:GLN:HB3	4:G:326:HOH:O	2.04	0.56
1:J:132:GLN:HE21	1:J:138:ARG:HH22	1.52	0.56
1:G:22:SER:O	1:G:54:ARG:NH2	2.39	0.56
1:B:3:LYS:NZ	1:B:223:TYR:O	2.39	0.56
1:E:27:LEU:O	1:E:31:THR:HG23	2.05	0.56
1:C:10:ALA:HB1	1:C:237:SER:HB2	1.88	0.55
1:I:92:VAL:C	1:I:93:LEU:HD12	2.27	0.55
1:I:214:VAL:HG21	1:I:231:PHE:CD1	2.41	0.55
1:J:1:MET:O	1:J:2:SER:OG	2.19	0.55
1:B:220:ARG:O	1:B:224:GLN:HG3	2.06	0.55
1:H:134:ARG:CZ	1:H:170:TRP:CZ2	2.90	0.55
1:I:13:LYS:NZ	1:I:97:GLU:OE2	2.31	0.55
1:E:220:ARG:O	1:E:224:GLN:HG2	2.07	0.55
1:H:215:ASN:H	1:H:218:ASN:ND2	2.05	0.55
1:G:46:VAL:CG2	1:H:82:ILE:HD11	2.38	0.54
1:H:16:GLY:HA3	1:H:21:LEU:HD11	1.88	0.54
1:K:21:LEU:O	1:K:25:ILE:HG23	2.08	0.54
1:H:3:LYS:NZ	1:H:223:TYR:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLU:CD	1:I:1:MET:HB3	2.25	0.54
1:E:55:LEU:HD21	1:E:60:PHE:HB3	1.89	0.53
1:G:154:LEU:HD21	1:G:162:VAL:HG21	1.88	0.53
1:L:116:ALA:HB1	1:L:121:PHE:HB2	1.90	0.53
1:C:141:VAL:O	1:C:145:THR:OG1	2.21	0.53
1:H:129:GLU:HG2	1:H:139:THR:HA	1.90	0.53
1:H:29:ASN:HA	1:H:57:HIS:HB2	1.91	0.53
1:H:79:SER:O	1:H:82:ILE:HG23	2.09	0.53
1:G:33:ILE:HB	1:G:59:LYS:HD3	1.91	0.52
1:A:20:SER:OG	3:A:302:PEG:H32	2.09	0.52
1:H:215:ASN:H	1:H:218:ASN:HD21	1.56	0.52
1:C:220:ARG:NH2	1:C:250:GLN:O	2.38	0.52
1:C:26:ASP:OD2	1:C:54:ARG:NH2	2.42	0.52
1:H:69:ALA:HA	1:H:80:LEU:HD12	1.92	0.52
1:L:191:ARG:NE	1:L:227:ASP:OD1	2.42	0.52
1:L:33:ILE:O	1:L:59:LYS:NZ	2.35	0.52
1:D:55:LEU:HD21	1:D:60:PHE:HB3	1.92	0.52
1:I:3:LYS:CE	1:I:226:ARG:O	2.58	0.52
1:L:129:GLU:OE2	1:L:134:ARG:NH1	2.43	0.52
1:G:214:VAL:CG2	1:G:214:VAL:O	2.58	0.51
1:I:35:HIS:CD2	1:I:250:GLN:HG2	2.45	0.51
1:A:55:LEU:HD21	1:A:60:PHE:HB3	1.91	0.51
1:L:130:THR:HA	1:L:169:VAL:HB	1.93	0.51
1:B:49:ALA:HB1	3:B:301:PEG:H42	1.91	0.51
1:L:144:LEU:HD13	1:L:193:TRP:HD1	1.76	0.51
1:G:240:PRO:O	1:G:243:VAL:HG12	2.10	0.51
1:C:215:ASN:HB2	1:C:241:GLU:OE2	2.10	0.51
1:G:79:SER:HB2	1:G:81:PRO:HD2	1.93	0.51
1:G:47:HIS:NE2	1:H:82:ILE:HD13	2.25	0.51
1:B:194:VAL:HG12	1:B:203:ALA:HB2	1.93	0.51
1:B:205:GLU:HG3	1:I:1:MET:HB3	1.83	0.51
1:L:144:LEU:HD13	1:L:193:TRP:CD1	2.46	0.51
1:L:28:PHE:O	1:L:31:THR:HG22	2.10	0.51
1:G:138:ARG:O	1:G:142:VAL:HG12	2.10	0.51
1:I:29:ASN:ND2	1:I:54:ARG:O	2.43	0.51
1:E:179:THR:HG23	1:E:181:GLN:H	1.77	0.50
1:L:233:VAL:HG13	1:L:237:SER:HB3	1.92	0.50
1:B:55:LEU:HD21	1:B:60:PHE:HB3	1.91	0.50
1:D:28:PHE:O	1:D:31:THR:HG22	2.11	0.50
1:F:110:ALA:HB1	1:F:153:LYS:HG3	1.94	0.50
1:C:13:LYS:CE	3:C:301:PEG:H31	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:201:ASP:N	1:K:201:ASP:OD1	2.45	0.50
1:C:220:ARG:NH1	1:C:248:ALA:O	2.40	0.50
1:F:187:HIS:ND1	1:F:227:ASP:O	2.42	0.50
1:J:1:MET:SD	1:J:204:GLY:HA2	2.51	0.50
1:K:55:LEU:HD21	1:K:60:PHE:HB3	1.94	0.49
1:F:42:ALA:HA	1:F:63:ALA:O	2.12	0.49
1:C:138:ARG:NH1	4:C:461:HOH:O	2.45	0.49
1:K:52:LYS:NZ	1:K:86:PHE:O	2.38	0.49
1:H:134:ARG:NE	1:H:170:TRP:CH2	2.81	0.49
1:B:156:LYS:HG3	1:I:226:ARG:CZ	2.42	0.49
1:H:235:GLY:N	2:H:301:SO4:O3	2.41	0.49
1:K:214:VAL:HG12	1:K:245:ILE:HD12	1.95	0.49
1:J:45:PHE:HA	1:J:48:LEU:HD22	1.93	0.49
1:K:220:ARG:O	1:K:224:GLN:HG2	2.13	0.49
1:K:45:PHE:HB2	1:L:45:PHE:HB2	1.95	0.49
1:C:47:HIS:HA	4:C:456:HOH:O	2.12	0.49
1:G:31:THR:HG21	1:G:243:VAL:HG23	1.95	0.49
1:G:33:ILE:HD13	1:G:59:LYS:HD3	1.95	0.49
1:B:156:LYS:HE3	1:B:201:ASP:OD1	2.13	0.49
1:G:127:ILE:HD12	1:G:143:VAL:HG13	1.94	0.49
1:G:195:SER:HA	1:G:199:GLY:O	2.13	0.48
1:I:7:ILE:HG12	1:I:38:GLN:HB3	1.95	0.48
1:H:130:THR:N	1:H:133:GLU:OE1	2.36	0.48
1:F:55:LEU:HD21	1:F:60:PHE:HB3	1.94	0.48
1:D:79:SER:HB2	1:D:81:PRO:HD2	1.94	0.48
1:K:186:ALA:O	1:K:190:ILE:HG12	2.13	0.48
1:F:33:ILE:HB	1:F:59:LYS:HD2	1.95	0.48
1:B:1:MET:SD	1:I:156:LYS:HG2	2.54	0.48
1:K:25:ILE:HG13	1:K:26:ASP:N	2.27	0.48
1:J:220:ARG:HD2	1:J:221:THR:N	2.28	0.47
1:K:117:VAL:HG11	1:K:158:ASP:HB3	1.96	0.47
1:K:17:SER:HB2	1:L:85:ASP:OD1	2.13	0.47
1:H:168:PRO:CD	1:H:211:GLY:O	2.62	0.47
1:H:218:ASN:H	1:H:218:ASN:HD22	1.62	0.47
1:F:32:SER:O	1:F:247:LYS:NZ	2.47	0.47
1:E:201:ASP:N	1:E:201:ASP:OD2	2.46	0.47
1:K:191:ARG:NH1	1:K:206:LEU:O	2.37	0.47
1:H:170:TRP:CG	1:H:170:TRP:O	2.59	0.47
1:J:244:ASP:O	1:J:247:LYS:HD2	2.15	0.47
1:A:138:ARG:NH2	1:C:196:SER:O	2.47	0.47
1:I:24:LEU:HD21	1:I:238:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:129:GLU:OE2	1:L:170:TRP:NE1	2.47	0.47
1:G:33:ILE:O	1:G:59:LYS:NZ	2.44	0.47
1:H:184:GLN:NE2	1:H:227:ASP:OD2	2.37	0.47
1:H:138:ARG:O	1:H:142:VAL:HG12	2.14	0.47
1:H:169:VAL:C	1:H:171:ALA:N	2.68	0.47
1:G:184:GLN:NE2	1:G:226:ARG:HB3	2.29	0.46
1:B:33:ILE:HD13	1:B:246:ILE:HG21	1.95	0.46
1:H:18:GLN:O	1:H:22:SER:HB2	2.15	0.46
1:H:178:ALA:N	1:H:182:GLN:OE1	2.48	0.46
1:F:33:ILE:O	1:F:59:LYS:HE3	2.15	0.46
1:G:168:PRO:HG2	4:G:327:HOH:O	2.15	0.46
1:I:55:LEU:HD21	1:I:60:PHE:HB3	1.98	0.46
1:F:233:VAL:HB	1:F:237:SER:HB3	1.98	0.46
1:B:220:ARG:HH12	1:B:250:GLN:C	2.19	0.46
1:G:102:TYR:CZ	1:H:77:GLU:HG3	2.51	0.46
1:C:172:ILE:HA	1:C:173:GLY:HA2	1.59	0.46
1:H:50:MET:N	4:H:418:HOH:O	2.49	0.46
1:F:80:LEU:HB2	1:F:81:PRO:HD3	1.98	0.46
1:G:55:LEU:HD21	1:G:60:PHE:HB3	1.98	0.46
1:I:156:LYS:NZ	1:I:201:ASP:OD1	2.42	0.46
1:J:48:LEU:HB3	1:J:86:PHE:HE2	1.81	0.46
1:L:26:ASP:OD1	1:L:54:ARG:NH2	2.44	0.46
1:H:129:GLU:HG3	1:H:143:VAL:HG23	1.97	0.46
1:J:152:LYS:HE2	1:J:153:LYS:NZ	2.28	0.45
1:J:181:GLN:HB2	1:J:181:GLN:HE21	1.51	0.45
1:L:179:THR:OG1	1:L:182:GLN:HB2	2.16	0.45
1:G:57:HIS:CD2	1:G:58:PRO:HD2	2.52	0.45
1:A:220:ARG:O	1:A:224:GLN:HG3	2.15	0.45
1:I:92:VAL:O	1:I:93:LEU:HD12	2.15	0.45
1:L:33:ILE:HD13	1:L:246:ILE:HG21	1.99	0.45
1:C:132:GLN:HE21	1:C:132:GLN:HB3	1.65	0.45
1:H:55:LEU:HD11	1:H:60:PHE:CB	2.47	0.45
1:I:24:LEU:HA	1:I:24:LEU:HD13	1.74	0.45
1:J:144:LEU:HD13	1:J:193:TRP:CD1	2.52	0.45
1:F:180:PRO:HA	1:F:222:LEU:HD23	1.99	0.45
1:J:215:ASN:ND2	1:J:217:LYS:HB2	2.30	0.45
1:B:191:ARG:NE	1:B:227:ASP:OD1	2.46	0.45
1:B:205:GLU:CG	1:I:1:MET:CB	2.60	0.45
1:G:46:VAL:HG12	1:H:48:LEU:HD12	1.98	0.45
1:F:193:TRP:CZ3	1:F:198:ILE:HD11	2.52	0.44
1:B:57:HIS:HB3	1:B:60:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:48:LEU:HB3	1:J:86:PHE:CE2	2.53	0.44
1:L:134:ARG:HD2	1:L:170:TRP:CD1	2.52	0.44
1:I:75:THR:HG23	1:J:65:GLN:HB3	1.99	0.44
1:K:79:SER:HB2	1:K:81:PRO:HD2	1.99	0.44
1:L:134:ARG:HH21	1:L:182:GLN:HE21	1.65	0.44
1:G:184:GLN:HE22	1:G:226:ARG:HB3	1.82	0.44
1:E:179:THR:HG23	1:E:181:GLN:N	2.32	0.44
1:G:156:LYS:NZ	1:G:198:ILE:HA	2.33	0.44
1:I:168:PRO:HD2	1:I:211:GLY:O	2.18	0.44
1:L:50:MET:HG3	1:L:51:THR:N	2.33	0.44
1:J:184:GLN:NE2	1:J:227:ASP:OD2	2.41	0.44
1:K:45:PHE:CB	1:L:45:PHE:HB2	2.48	0.44
1:C:50:MET:HG3	1:C:54:ARG:HD3	2.00	0.44
1:F:48:LEU:O	1:F:52:LYS:HB2	2.18	0.44
1:G:127:ILE:HB	1:G:146:GLN:OE1	2.18	0.44
1:I:155:LYS:HG2	1:I:158:ASP:OD2	2.18	0.44
1:I:33:ILE:HD12	1:I:246:ILE:HG21	2.00	0.44
1:J:70:LYS:HB3	1:J:70:LYS:HE2	1.91	0.44
1:K:129:GLU:OE2	1:K:170:TRP:NE1	2.50	0.44
1:E:24:LEU:HD21	1:E:238:LEU:HA	1.99	0.43
1:F:187:HIS:HB3	1:F:227:ASP:HB3	2.00	0.43
1:K:14:CYS:SG	1:L:79:SER:HB3	2.59	0.43
1:G:132:GLN:HE21	1:G:132:GLN:HB2	1.50	0.43
1:L:164:ILE:HG12	1:L:206:LEU:HD11	2.01	0.43
1:D:3:LYS:HB3	4:D:424:HOH:O	2.18	0.43
1:H:63:ALA:HA	1:H:90:TRP:O	2.18	0.43
1:J:132:GLN:NE2	1:J:138:ARG:HH22	2.17	0.43
3:B:301:PEG:O1	3:B:301:PEG:H41	2.19	0.43
4:A:496:HOH:O	1:C:197:LYS:HE2	2.19	0.43
1:C:35:HIS:CD2	1:C:37:VAL:HG23	2.52	0.43
1:J:244:ASP:HA	1:J:247:LYS:NZ	2.33	0.43
1:K:184:GLN:NE2	1:K:227:ASP:OD2	2.30	0.43
1:G:41:VAL:HG23	1:G:62:ILE:HG22	2.01	0.43
1:H:134:ARG:NE	1:H:170:TRP:CZ2	2.87	0.43
1:F:212:GLY:O	1:F:214:VAL:HG23	2.18	0.43
1:L:7:ILE:HG12	1:L:38:GLN:HB3	2.01	0.43
1:C:201:ASP:N	1:C:201:ASP:OD2	2.51	0.43
1:D:167:GLU:HG3	1:D:167:GLU:O	2.18	0.43
1:E:179:THR:CG2	1:E:182:GLN:H	2.32	0.43
1:G:22:SER:CB	1:G:54:ARG:HH12	2.32	0.43
1:G:241:GLU:HA	1:G:244:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:PHE:CE2	1:G:246:ILE:HD11	2.53	0.43
1:I:70:LYS:HB3	1:I:70:LYS:HE3	1.80	0.43
1:C:205:GLU:HB2	4:C:463:HOH:O	2.19	0.42
1:F:158:ASP:OD1	4:F:316:HOH:O	2.21	0.42
1:G:193:TRP:O	1:G:197:LYS:HG2	2.19	0.42
1:K:109:VAL:O	1:K:113:VAL:HG23	2.18	0.42
1:B:144:LEU:HA	1:B:147:ILE:HG22	2.01	0.42
1:K:187:HIS:CD2	1:K:228:VAL:HG22	2.54	0.42
1:D:191:ARG:NE	1:D:227:ASP:OD1	2.49	0.42
1:G:220:ARG:HE	1:G:224:GLN:HE21	1.68	0.42
1:G:25:ILE:HG22	1:G:29:ASN:ND2	2.34	0.42
1:H:195:SER:HB3	1:H:200:ALA:HA	2.01	0.42
1:G:46:VAL:HG13	1:H:45:PHE:HB3	2.01	0.42
1:I:3:LYS:HB3	1:I:4:PRO:HD2	2.01	0.42
1:A:24:LEU:HD22	3:A:302:PEG:H12	2.00	0.42
1:K:131:LEU:HA	1:K:170:TRP:HB3	2.01	0.42
1:G:220:ARG:NE	1:G:224:GLN:HE21	2.17	0.42
1:G:220:ARG:NH2	1:G:224:GLN:HE21	2.17	0.42
1:B:49:ALA:CB	3:B:301:PEG:H42	2.48	0.42
1:K:33:ILE:HB	1:K:59:LYS:HD2	2.00	0.42
1:L:133:GLU:HB3	1:L:138:ARG:HB3	2.01	0.42
1:D:220:ARG:O	1:D:224:GLN:HG2	2.20	0.42
1:F:177:VAL:HG11	1:F:213:SER:O	2.19	0.42
1:G:134:ARG:HA	1:G:139:THR:OG1	2.20	0.42
1:J:149:ALA:O	1:J:152:LYS:HG2	2.20	0.42
1:A:155:LYS:HD3	1:A:155:LYS:HA	1.69	0.42
1:B:130:THR:HG23	1:B:133:GLU:OE1	2.20	0.42
1:E:117:VAL:HG11	1:E:158:ASP:HB3	2.01	0.42
1:G:214:VAL:HG23	1:G:214:VAL:O	2.20	0.42
1:K:105:THR:O	1:K:109:VAL:HG23	2.19	0.42
1:A:237:SER:HA	1:A:242:PHE:HB2	2.02	0.41
1:F:117:VAL:HG11	1:F:158:ASP:HB3	2.01	0.41
1:L:18:GLN:O	1:L:22:SER:HB2	2.19	0.41
1:C:152:LYS:HB2	1:C:152:LYS:HE2	1.83	0.41
1:G:116:ALA:O	1:G:121:PHE:HB2	2.20	0.41
1:H:155:LYS:HG2	1:H:158:ASP:OD2	2.20	0.41
1:L:117:VAL:HG13	1:L:161:LYS:HB2	2.01	0.41
1:A:117:VAL:HG11	1:A:158:ASP:HB3	2.02	0.41
1:C:131:LEU:HA	1:C:170:TRP:HB3	2.03	0.41
1:H:170:TRP:C	1:H:170:TRP:CD1	2.93	0.41
1:H:42:ALA:HA	1:H:63:ALA:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:GLU:OE2	1:H:73:ALA:HB1	2.19	0.41
1:I:5:GLN:HA	1:I:6:PRO:HD2	1.94	0.41
1:J:191:ARG:HE	1:J:227:ASP:HB3	1.86	0.41
1:A:191:ARG:NE	1:A:227:ASP:OD1	2.52	0.41
1:B:193:TRP:CE2	1:B:197:LYS:HG2	2.56	0.41
1:C:220:ARG:HA	1:C:220:ARG:HD2	1.74	0.41
1:C:62:ILE:HG22	1:C:88:VAL:HG13	2.02	0.41
1:E:80:LEU:HB2	1:E:81:PRO:HD3	2.01	0.41
1:G:18:GLN:NE2	1:H:85:ASP:O	2.53	0.41
1:D:24:LEU:HD21	1:D:238:LEU:HA	2.03	0.41
1:J:21:LEU:HB2	1:J:50:MET:HE1	2.02	0.41
1:L:7:ILE:O	1:L:230:GLY:HA3	2.21	0.41
1:H:214:VAL:HG11	1:H:231:PHE:CD1	2.56	0.41
1:G:239:LYS:HB3	1:G:240:PRO:HD2	2.03	0.41
1:H:129:GLU:CD	1:H:170:TRP:HZ3	2.23	0.41
1:J:3:LYS:HE2	1:J:226:ARG:O	2.20	0.41
1:K:131:LEU:O	1:K:135:GLU:HG2	2.21	0.41
1:K:239:LYS:HB3	4:K:410:HOH:O	2.20	0.41
1:H:49:ALA:HB2	1:H:86:PHE:HZ	1.85	0.41
1:C:4:PRO:HB2	1:C:207:ARG:HD2	2.03	0.41
1:H:191:ARG:NE	1:H:227:ASP:OD1	2.48	0.41
1:K:166:TYR:HB3	1:K:187:HIS:HE1	1.86	0.41
1:L:16:GLY:HA3	1:L:21:LEU:HD11	2.03	0.41
1:J:55:LEU:HD21	1:J:60:PHE:HB3	2.03	0.40
1:L:62:ILE:HD11	1:L:88:VAL:HG22	2.03	0.40
1:G:59:LYS:HE3	1:G:59:LYS:HB2	1.94	0.40
1:I:155:LYS:HG2	1:I:158:ASP:CG	2.41	0.40
1:E:144:LEU:HD23	1:E:144:LEU:HA	1.83	0.40
1:I:3:LYS:HA	1:I:4:PRO:HD3	1.83	0.40
1:J:215:ASN:HD21	1:J:217:LYS:HB2	1.86	0.40
1:J:235:GLY:C	1:J:237:SER:N	2.75	0.40
1:B:181:GLN:N	1:B:181:GLN:OE1	2.51	0.40
1:F:52:LYS:HA	1:F:62:ILE:CD1	2.52	0.40
1:G:234:GLY:O	1:G:237:SER:OG	2.26	0.40
1:G:31:THR:HG22	1:G:33:ILE:HG13	2.03	0.40
1:J:128:GLY:HA3	1:J:167:GLU:O	2.20	0.40
1:G:220:ARG:HH21	1:G:224:GLN:HE21	1.70	0.40
1:H:131:LEU:CA	1:H:170:TRP:HB3	2.52	0.40
1:I:134:ARG:HD3	1:I:170:TRP:NE1	2.37	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	248/250 (99%)	243 (98%)	5 (2%)	0	100	100
1	B	241/250 (96%)	237 (98%)	4 (2%)	0	100	100
1	C	244/250 (98%)	237 (97%)	7 (3%)	0	100	100
1	D	248/250 (99%)	245 (99%)	3 (1%)	0	100	100
1	E	248/250 (99%)	240 (97%)	8 (3%)	0	100	100
1	F	245/250 (98%)	240 (98%)	5 (2%)	0	100	100
1	G	241/250 (96%)	231 (96%)	10 (4%)	0	100	100
1	H	239/250 (96%)	228 (95%)	11 (5%)	0	100	100
1	I	243/250 (97%)	231 (95%)	12 (5%)	0	100	100
1	J	245/250 (98%)	237 (97%)	8 (3%)	0	100	100
1	K	242/250 (97%)	232 (96%)	10 (4%)	0	100	100
1	L	242/250 (97%)	236 (98%)	6 (2%)	0	100	100
All	All	2926/3000 (98%)	2837 (97%)	89 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	197/197 (100%)	193 (98%)	4 (2%)	55	72
1	B	194/197 (98%)	191 (98%)	3 (2%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	196/197 (100%)	184 (94%)	12 (6%)	18	25
1	D	197/197 (100%)	194 (98%)	3 (2%)	65	79
1	E	196/197 (100%)	192 (98%)	4 (2%)	55	72
1	F	196/197 (100%)	187 (95%)	9 (5%)	27	38
1	G	193/197 (98%)	183 (95%)	10 (5%)	23	32
1	H	191/197 (97%)	178 (93%)	13 (7%)	16	21
1	I	195/197 (99%)	192 (98%)	3 (2%)	65	79
1	J	196/197 (100%)	182 (93%)	14 (7%)	14	19
1	K	195/197 (99%)	183 (94%)	12 (6%)	18	25
1	L	195/197 (99%)	183 (94%)	12 (6%)	18	25
All	All	2341/2364 (99%)	2242 (96%)	99 (4%)	30	42

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	107	GLU
1	A	119	SER
1	A	132	GLN
1	B	1	MET
1	B	207	ARG
1	B	250	GLN
1	C	1	MET
1	C	19	GLN
1	C	32	SER
1	C	62	ILE
1	C	132	GLN
1	C	156	LYS
1	C	177	VAL
1	C	197	LYS
1	C	207	ARG
1	C	222	LEU
1	C	226	ARG
1	C	247	LYS
1	D	1	MET
1	D	54	ARG
1	D	152	LYS
1	E	1	MET

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Mol	Chain	Res	Type
1	E	2	SER
1	E	174	THR
1	E	196	SER
1	F	50	MET
1	F	53	GLU
1	F	155	LYS
1	F	172	ILE
1	F	176	LYS
1	F	197	LYS
1	F	207	ARG
1	F	213	SER
1	F	241	GLU
1	G	2	SER
1	G	132	GLN
1	G	135	GLU
1	G	155	LYS
1	G	169	VAL
1	G	179	THR
1	G	196	SER
1	G	209	LEU
1	G	218	ASN
1	G	221	THR
1	H	19	GLN
1	H	31	THR
1	H	70	LYS
1	H	82	ILE
1	H	129	GLU
1	H	132	GLN
1	H	142	VAL
1	H	154	LEU
1	H	195	SER
1	H	207	ARG
1	H	218	ASN
1	H	233	VAL
1	H	241	GLU
1	I	1	MET
1	I	2	SER
1	I	24	LEU
1	J	1	MET
1	J	19	GLN
1	J	30	SER
1	J	46	VAL

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Mol	Chain	Res	Type
1	J	48	LEU
1	J	53	GLU
1	J	89	ASN
1	J	132	GLN
1	J	181	GLN
1	J	192	SER
1	J	197	LYS
1	J	207	ARG
1	J	221	THR
1	J	247	LYS
1	K	1	MET
1	K	35	HIS
1	K	51	THR
1	K	53	GLU
1	K	107	GLU
1	K	144	LEU
1	K	147	ILE
1	K	172	ILE
1	K	181	GLN
1	K	207	ARG
1	K	222	LEU
1	K	224	GLN
1	L	1	MET
1	L	22	SER
1	L	41	VAL
1	L	62	ILE
1	L	84	LYS
1	L	89	ASN
1	L	138	ARG
1	L	141	VAL
1	L	177	VAL
1	L	182	GLN
1	L	214	VAL
1	L	218	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	57	HIS
1	A	224	GLN
1	A	225	GLN

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Mol	Chain	Res	Type
1	B	132	GLN
1	C	132	GLN
1	D	187	HIS
1	E	34	ASN
1	F	18	GLN
1	G	18	GLN
1	G	29	ASN
1	G	57	HIS
1	G	132	GLN
1	G	182	GLN
1	G	224	GLN
1	H	18	GLN
1	H	218	ASN
1	I	35	HIS
1	I	89	ASN
1	J	181	GLN
1	J	250	GLN
1	K	57	HIS
1	K	187	HIS
1	L	47	HIS
1	L	218	ASN
1	L	229	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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	SO4	D	301	-	4,4,4	0.22	0	6,6,6	0.13	0
2	SO4	A	301	-	4,4,4	0.26	0	6,6,6	0.14	0
2	SO4	D	302	-	4,4,4	0.17	0	6,6,6	0.12	0
2	SO4	K	301	-	4,4,4	0.18	0	6,6,6	0.11	0
2	SO4	H	301	-	4,4,4	0.18	0	6,6,6	0.25	0
3	PEG	B	301	-	6,6,6	0.60	0	5,5,5	0.43	0
3	PEG	B	302	-	6,6,6	0.61	0	5,5,5	0.33	0
3	PEG	A	302	-	6,6,6	0.61	0	5,5,5	0.41	0
3	PEG	C	301	-	6,6,6	0.66	0	5,5,5	0.38	0
3	PEG	E	301	-	6,6,6	0.65	0	5,5,5	0.38	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	B	302	-	-	2/4/4/4	-
3	PEG	E	301	-	-	2/4/4/4	-
3	PEG	B	301	-	-	3/4/4/4	-
3	PEG	C	301	-	-	2/4/4/4	-
3	PEG	A	302	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	PEG	C4-C3-O2-C2
3	E	301	PEG	C1-C2-O2-C3
3	B	302	PEG	C4-C3-O2-C2
3	A	302	PEG	O1-C1-C2-O2
3	C	301	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	B	301	PEG	O2-C3-C4-O4
3	A	302	PEG	O2-C3-C4-O4
3	C	301	PEG	O1-C1-C2-O2
3	E	301	PEG	O2-C3-C4-O4
3	B	301	PEG	C1-C2-O2-C3
3	B	302	PEG	C1-C2-O2-C3
3	B	301	PEG	C4-C3-O2-C2

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	SO4	1	0
3	B	301	PEG	5	0
3	B	302	PEG	1	0
3	A	302	PEG	3	0
3	C	301	PEG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	250/250 (100%)	-0.14	0 100 100	8, 17, 33, 42	0
1	B	245/250 (98%)	-0.13	1 (0%) 92 95	9, 20, 38, 55	0
1	C	248/250 (99%)	-0.06	1 (0%) 92 95	14, 27, 48, 64	0
1	D	250/250 (100%)	-0.14	2 (0%) 86 89	11, 22, 38, 49	0
1	E	250/250 (100%)	-0.11	4 (1%) 72 77	13, 23, 38, 67	0
1	F	249/250 (99%)	0.40	14 (5%) 24 30	19, 34, 51, 71	0
1	G	245/250 (98%)	0.70	26 (10%) 6 8	17, 40, 64, 70	0
1	H	243/250 (97%)	0.72	24 (9%) 7 10	18, 41, 61, 68	0
1	I	247/250 (98%)	0.17	10 (4%) 38 45	19, 34, 66, 72	0
1	J	249/250 (99%)	0.82	29 (11%) 4 6	25, 48, 65, 75	0
1	K	246/250 (98%)	0.98	46 (18%) 1 1	31, 55, 69, 83	0
1	L	246/250 (98%)	0.65	21 (8%) 10 14	31, 49, 69, 76	0
All	All	2968/3000 (98%)	0.32	178 (5%) 21 28	8, 34, 62, 83	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	190	ILE	6.4
1	H	21	LEU	5.2
1	L	138	ARG	5.1
1	G	51	THR	5.0
1	H	243	VAL	4.8
1	K	183	ALA	4.7
1	F	190	ILE	4.5
1	G	33	ILE	4.4
1	J	233	VAL	4.4
1	F	22	SER	4.3
1	K	144	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	J	214	VAL	4.2
1	G	240	PRO	4.2
1	J	32	SER	4.2
1	H	19	GLN	4.2
1	G	62	ILE	4.2
1	K	121	PHE	4.1
1	K	7	ILE	4.0
1	G	23	GLU	4.0
1	K	172	ILE	3.9
1	J	190	ILE	3.9
1	K	37	VAL	3.9
1	G	31	THR	3.8
1	H	28	PHE	3.8
1	J	232	LEU	3.7
1	H	62	ILE	3.7
1	G	238	LEU	3.7
1	L	32	SER	3.7
1	K	143	VAL	3.7
1	K	214	VAL	3.6
1	K	204	GLY	3.6
1	K	50	MET	3.5
1	L	30	SER	3.5
1	H	34	ASN	3.5
1	H	26	ASP	3.4
1	G	137	GLY	3.4
1	K	177	VAL	3.4
1	H	142	VAL	3.4
1	L	23	GLU	3.4
1	J	1	MET	3.3
1	J	240	PRO	3.3
1	J	7	ILE	3.3
1	H	31	THR	3.3
1	I	51	THR	3.2
1	K	211	GLY	3.2
1	J	216	GLY	3.2
1	B	1	MET	3.2
1	J	60	PHE	3.1
1	K	193	TRP	3.1
1	L	132	GLN	3.1
1	G	63	ALA	3.1
1	H	16	GLY	3.1
1	D	216	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	170	TRP	3.0
1	J	177	VAL	3.0
1	H	30	SER	3.0
1	J	188	ALA	2.9
1	H	240	PRO	2.9
1	L	239	LYS	2.9
1	K	194	VAL	2.9
1	L	1	MET	2.9
1	G	19	GLN	2.9
1	C	1	MET	2.9
1	K	1	MET	2.9
1	K	191	ARG	2.9
1	K	127	ILE	2.8
1	L	31	THR	2.8
1	G	55	LEU	2.8
1	H	24	LEU	2.8
1	K	30	SER	2.8
1	H	61	VAL	2.8
1	G	138	ARG	2.8
1	G	214	VAL	2.8
1	F	140	ALA	2.7
1	G	88	VAL	2.7
1	H	219	ALA	2.7
1	H	22	SER	2.7
1	L	147	ILE	2.7
1	J	178	ALA	2.7
1	K	198	ILE	2.7
1	H	134	ARG	2.7
1	K	192	SER	2.7
1	E	177	VAL	2.7
1	I	176	LYS	2.6
1	F	177	VAL	2.6
1	J	46	VAL	2.6
1	I	89	ASN	2.6
1	F	219	ALA	2.6
1	K	220	ARG	2.6
1	K	36	ASP	2.6
1	K	32	SER	2.6
1	K	216	GLY	2.6
1	E	174	THR	2.6
1	F	11	ASN	2.6
1	K	187	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	7	ILE	2.6
1	K	189	LEU	2.5
1	K	205	GLU	2.5
1	G	246	ILE	2.5
1	I	175	GLY	2.5
1	I	171	ALA	2.5
1	G	133	GLU	2.5
1	J	219	ALA	2.5
1	F	178	ALA	2.4
1	K	88	VAL	2.4
1	K	231	PHE	2.4
1	J	231	PHE	2.4
1	L	34	ASN	2.4
1	J	175	GLY	2.4
1	F	144	LEU	2.4
1	L	177	VAL	2.4
1	G	27	LEU	2.4
1	K	162	VAL	2.4
1	L	37	VAL	2.4
1	F	166	TYR	2.4
1	K	35	HIS	2.4
1	G	50	MET	2.4
1	E	175	GLY	2.3
1	J	228	VAL	2.3
1	J	40	VAL	2.3
1	J	242	PHE	2.3
1	G	32	SER	2.3
1	G	156	LYS	2.3
1	K	60	PHE	2.3
1	J	215	ASN	2.3
1	K	240	PRO	2.3
1	L	238	LEU	2.3
1	K	250	GLN	2.3
1	E	1	MET	2.3
1	H	226	ARG	2.3
1	K	186	ALA	2.3
1	L	19	GLN	2.3
1	L	245	ILE	2.3
1	I	55	LEU	2.2
1	F	37	VAL	2.2
1	K	242	PHE	2.2
1	G	21	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	86	PHE	2.2
1	K	147	ILE	2.2
1	L	154	LEU	2.2
1	L	137	GLY	2.2
1	K	33	ILE	2.2
1	F	141	VAL	2.2
1	G	20	SER	2.2
1	H	37	VAL	2.2
1	H	186	ALA	2.2
1	I	235	GLY	2.2
1	H	250	GLN	2.2
1	K	84	LYS	2.1
1	I	88	VAL	2.1
1	J	54	ARG	2.1
1	F	4	PRO	2.1
1	I	1	MET	2.1
1	J	41	VAL	2.1
1	J	202	VAL	2.1
1	H	17	SER	2.1
1	J	63	ALA	2.1
1	L	242	PHE	2.1
1	I	2	SER	2.1
1	J	173	GLY	2.1
1	G	147	ILE	2.1
1	J	135	GLU	2.1
1	G	140	ALA	2.1
1	K	228	VAL	2.1
1	K	74	PHE	2.1
1	G	47	HIS	2.1
1	H	59	LYS	2.1
1	K	165	ALA	2.1
1	K	159	TRP	2.1
1	L	60	PHE	2.1
1	K	227	ASP	2.0
1	J	246	ILE	2.0
1	H	53	GLU	2.0
1	D	174	THR	2.0
1	K	8	ALA	2.0
1	L	2	SER	2.0
1	J	156	LYS	2.0
1	F	250	GLN	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. 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(\AA^2)	Q<0.9
3	PEG	C	301	7/7	0.76	0.23	27,31,40,42	0
3	PEG	B	302	7/7	0.77	0.30	25,28,32,37	0
3	PEG	B	301	7/7	0.78	0.47	24,25,34,37	0
2	SO4	K	301	5/5	0.79	0.27	47,52,60,69	0
2	SO4	H	301	5/5	0.86	0.18	59,61,62,62	0
3	PEG	A	302	7/7	0.86	0.32	25,27,30,34	0
2	SO4	D	301	5/5	0.86	0.34	43,45,54,69	0
3	PEG	E	301	7/7	0.86	0.15	24,36,37,41	0
2	SO4	A	301	5/5	0.94	0.20	25,30,40,42	0
2	SO4	D	302	5/5	0.97	0.15	31,31,34,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.