



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:09 AM UTC

PDB ID : 4YXQ / pdb_00004yxq
Title : PksG, a HMG-CoA Synthase from *Bacillus subtilis*
Authors : Nair, A.V.; Race, P.R.; Till, M.
Deposited on : 2015-03-23
Resolution : 2.47 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

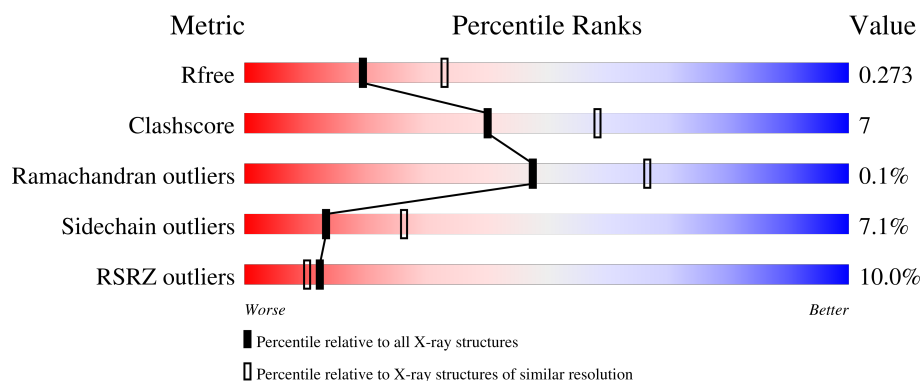
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	420	6% 82%12% . .
1	B	420	13% 79%13% . .
1	C	420	9% 81%12% . .
1	D	420	10% 81%11% . .

2 Entry composition [i](#)

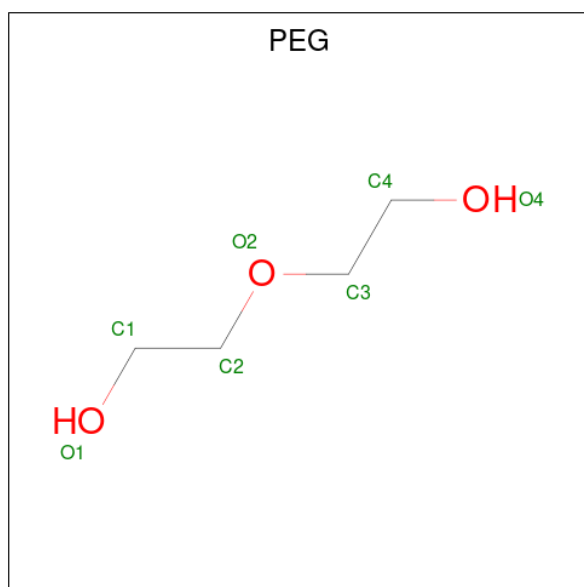
There are 3 unique types of molecules in this entry. The entry contains 12938 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polyketide biosynthesis 3-hydroxy-3-methylglutaryl-ACP synthase PksG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3170	2014	533	599	24			
1	B	402	Total	C	N	O	S	0	0	0
			3102	1966	521	590	25			
1	C	407	Total	C	N	O	S	0	0	0
			3178	2018	534	602	24			
1	D	402	Total	C	N	O	S	0	0	0
			3110	1971	525	590	24			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		

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

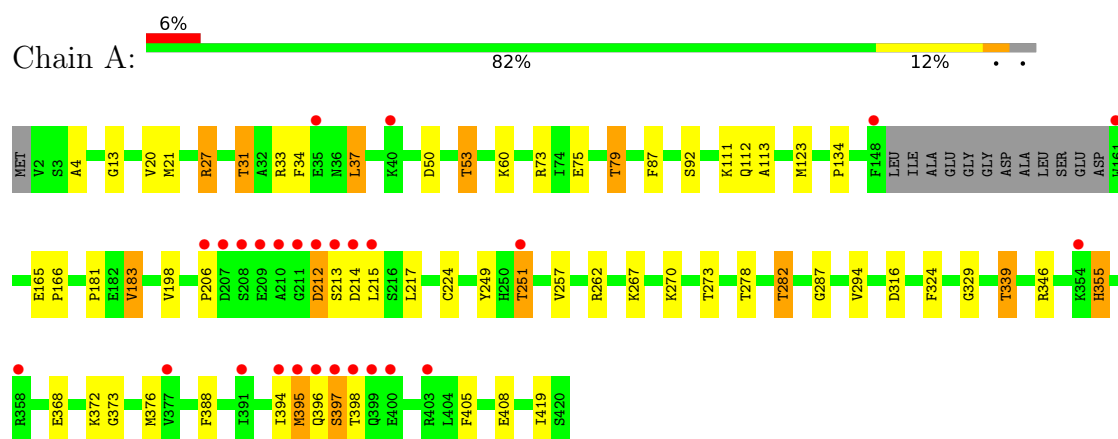
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	89	Total	O	0	0
			89	89		
3	B	85	Total	O	0	0
			85	85		
3	C	95	Total	O	0	0
			95	95		
3	D	88	Total	O	0	0
			88	88		

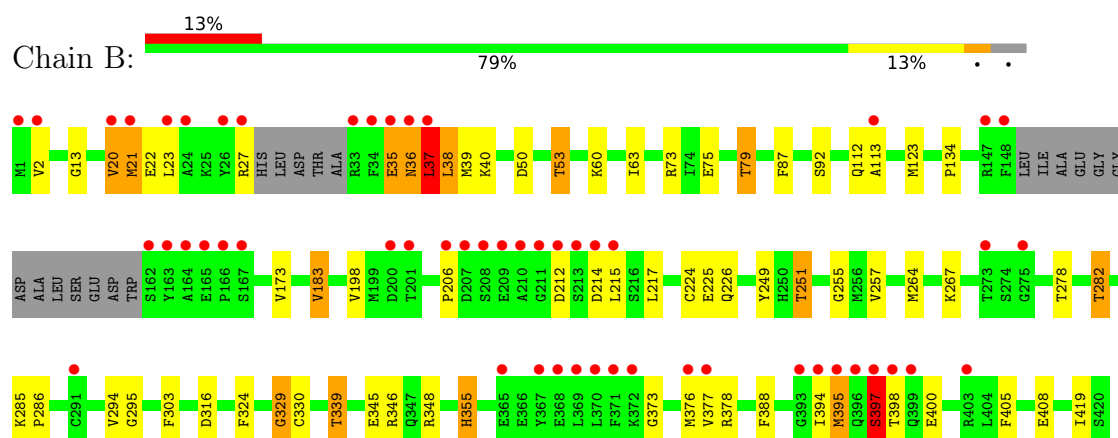
3 Residue-property plots

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.

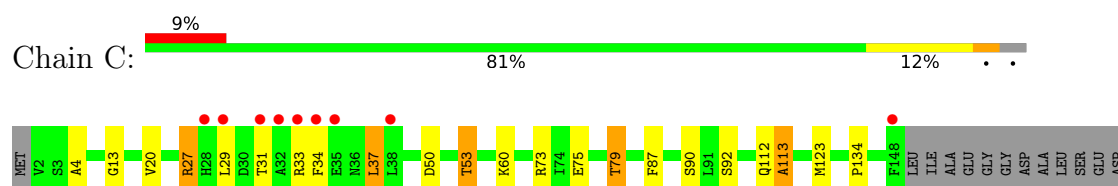
- Molecule 1: Polyketide biosynthesis 3-hydroxy-3-methylglutaryl-ACP synthase PksG

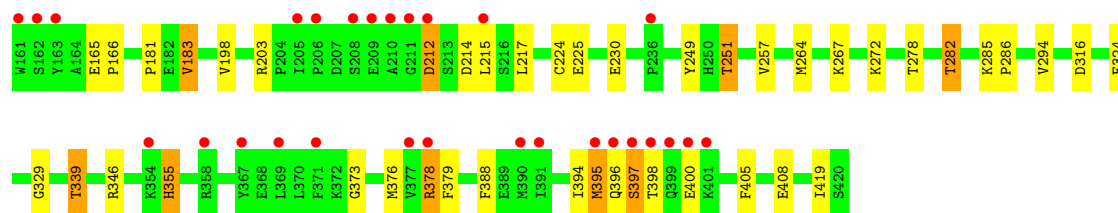


- Molecule 1: Polyketide biosynthesis 3-hydroxy-3-methylglutaryl-ACP synthase PksG

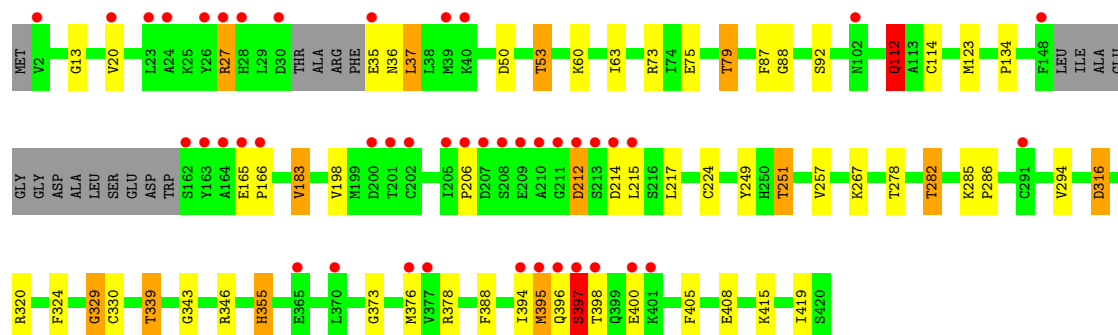
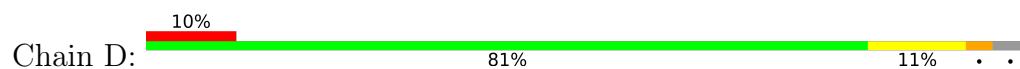


- Molecule 1: Polyketide biosynthesis 3-hydroxy-3-methylglutaryl-ACP synthase PksG





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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.62Å 122.04Å 198.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.74 – 2.47 63.74 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.74-2.47) 99.9 (63.74-2.48)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.226 , 0.271 0.229 , 0.273	Depositor DCC
R_{free} test set	3310 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12938	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7294e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.80	0/3238	0.91	2/4370 (0.0%)
1	B	0.83	0/3164	0.97	7/4268 (0.2%)
1	C	0.80	0/3246	0.91	3/4380 (0.1%)
1	D	0.90	2/3172 (0.1%)	0.94	6/4277 (0.1%)
All	All	0.83	2/12820 (0.0%)	0.93	18/17295 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	343	GLY	C-N	17.21	1.56	1.33
1	D	112	GLN	C-O	-5.52	1.17	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	397	SER	N-CA-C	10.58	122.78	111.03
1	C	329	GLY	N-CA-C	9.19	123.41	113.58
1	A	329	GLY	N-CA-C	8.94	123.14	113.58
1	D	397	SER	N-CA-C	8.06	119.98	111.03
1	B	329	GLY	N-CA-C	7.50	121.60	113.58
1	D	329	GLY	N-CA-C	6.97	121.03	113.58
1	B	37	LEU	N-CA-C	6.66	121.60	107.67
1	B	397	SER	CB-CA-C	-6.32	101.15	110.95
1	B	378	ARG	N-CA-C	-5.89	100.10	109.23
1	D	316	ASP	N-CA-CB	5.70	118.49	110.12
1	D	37	LEU	N-CA-C	5.48	119.83	113.20
1	B	113	ALA	CB-CA-C	-5.29	110.50	116.63
1	C	378	ARG	N-CA-C	-5.24	100.77	108.99
1	A	113	ALA	CB-CA-C	-5.22	110.57	116.63
1	C	113	ALA	CB-CA-C	-5.11	110.70	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	GLU	CB-CA-C	-5.11	102.80	110.92
1	D	378	ARG	N-CA-C	-5.03	101.09	108.99
1	D	397	SER	CB-CA-C	-5.03	103.16	110.95

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	3170	0	3088	41	0
1	B	3102	0	3013	52	0
1	C	3178	0	3098	44	0
1	D	3110	0	3031	39	0
2	B	7	0	10	0	0
2	D	14	0	20	2	0
3	A	89	0	0	7	0
3	B	85	0	0	3	0
3	C	95	0	0	2	0
3	D	88	0	0	2	0
All	All	12938	0	12260	165	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 (165) 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:20:VAL:HG12	1:B:40:LYS:O	1.56	1.06
1:B:20:VAL:HG12	1:B:40:LYS:C	1.89	0.97
1:B:37:LEU:HD13	1:B:255:GLY:HA3	1.47	0.95
1:A:251:THR:HB	1:A:257:VAL:HG21	1.50	0.93
1:D:123:MET:HA	1:D:123:MET:HE3	1.50	0.93
1:A:123:MET:HE3	1:A:123:MET:HA	1.51	0.92
1:A:398:THR:HG23	3:A:573:HOH:O	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:THR:HB	1:C:257:VAL:HG21	1.51	0.91
1:C:123:MET:HE3	1:C:123:MET:HA	1.52	0.91
1:B:123:MET:HE3	1:B:123:MET:HA	1.54	0.90
1:D:251:THR:HB	1:D:257:VAL:HG21	1.52	0.90
1:B:251:THR:HB	1:B:257:VAL:HG21	1.52	0.88
1:A:249:TYR:O	1:A:251:THR:HG22	1.81	0.81
1:B:35:GLU:O	1:B:36:ASN:C	2.22	0.80
1:D:249:TYR:O	1:D:251:THR:HG22	1.80	0.80
1:B:249:TYR:O	1:B:251:THR:HG22	1.80	0.79
1:B:20:VAL:CG1	1:B:40:LYS:C	2.56	0.79
1:C:249:TYR:O	1:C:251:THR:HG22	1.82	0.79
1:B:20:VAL:CG1	1:B:40:LYS:O	2.32	0.78
1:B:38:LEU:N	1:B:38:LEU:HD23	2.02	0.74
1:B:38:LEU:HD23	1:B:38:LEU:H	1.52	0.73
1:B:345:GLU:OE2	1:B:348:ARG:NH1	2.21	0.73
1:A:373:GLY:O	1:A:376:MET:HG2	1.90	0.71
1:C:373:GLY:O	1:C:376:MET:HG2	1.91	0.70
1:D:373:GLY:O	1:D:376:MET:HG2	1.92	0.69
1:B:21:MET:HG2	1:B:22:GLU:N	2.08	0.69
1:B:373:GLY:O	1:B:376:MET:HG2	1.92	0.69
1:A:73:ARG:NH2	1:A:134:PRO:O	2.29	0.66
1:D:320:ARG:CZ	2:D:501:PEG:H11	2.26	0.66
1:D:73:ARG:NH2	1:D:134:PRO:O	2.30	0.65
1:B:73:ARG:NH2	1:B:134:PRO:O	2.29	0.65
1:C:73:ARG:NH2	1:C:134:PRO:O	2.31	0.64
1:B:377:VAL:O	1:B:377:VAL:HG12	1.97	0.64
1:C:34:PHE:CZ	1:C:166:PRO:HG2	2.33	0.63
1:A:34:PHE:HA	1:A:37:LEU:HD22	1.82	0.61
1:B:183:VAL:O	1:B:339:THR:HB	2.03	0.59
1:B:39:MET:HE1	1:B:295:GLY:HA2	1.84	0.58
1:D:320:ARG:NH2	2:D:501:PEG:H11	2.18	0.58
1:A:262:ARG:NH1	3:A:503:HOH:O	2.36	0.58
1:D:183:VAL:O	1:D:339:THR:HB	2.03	0.58
1:B:63:ILE:HG22	3:B:615:HOH:O	2.02	0.58
1:A:273:THR:HG22	3:A:566:HOH:O	2.03	0.58
1:C:34:PHE:CE1	1:C:166:PRO:HG2	2.39	0.57
1:A:395:MET:HE1	1:A:405:PHE:CE2	2.39	0.57
1:A:183:VAL:O	1:A:339:THR:HB	2.04	0.57
1:D:50:ASP:H	1:D:53:THR:HB	1.70	0.57
1:B:50:ASP:H	1:B:53:THR:HB	1.70	0.57
1:B:226:GLN:NE2	3:B:601:HOH:O	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:MET:HE1	1:D:405:PHE:CE2	2.41	0.56
1:A:50:ASP:H	1:A:53:THR:HB	1.70	0.56
1:C:34:PHE:CZ	1:C:166:PRO:CG	2.88	0.56
1:C:50:ASP:H	1:C:53:THR:HB	1.71	0.56
1:C:183:VAL:O	1:C:339:THR:HB	2.05	0.56
1:C:395:MET:HE1	1:C:405:PHE:CE2	2.41	0.55
1:B:395:MET:HE1	1:B:405:PHE:CE2	2.43	0.54
1:C:13:GLY:H	1:C:355:HIS:CE1	2.24	0.54
1:B:13:GLY:H	1:B:355:HIS:CE1	2.26	0.54
1:C:13:GLY:H	1:C:355:HIS:HE1	1.56	0.54
1:C:388:PHE:CE2	1:C:419:ILE:HD11	2.43	0.54
1:A:287:GLY:HA3	3:A:540:HOH:O	2.07	0.54
1:A:388:PHE:CE2	1:A:419:ILE:HD11	2.43	0.54
1:D:114:CYS:SG	3:D:651:HOH:O	2.56	0.53
1:A:111:LYS:HB2	3:A:551:HOH:O	2.08	0.53
1:B:388:PHE:CE2	1:B:419:ILE:HD11	2.43	0.53
1:B:73:ARG:NH1	1:B:75:GLU:OE2	2.42	0.53
1:D:388:PHE:CE2	1:D:419:ILE:HD11	2.44	0.53
1:B:13:GLY:H	1:B:355:HIS:HE1	1.56	0.53
1:B:123:MET:HA	1:B:123:MET:CE	2.35	0.53
1:D:73:ARG:NH1	1:D:75:GLU:OE2	2.42	0.52
1:D:13:GLY:H	1:D:355:HIS:CE1	2.27	0.52
1:D:13:GLY:H	1:D:355:HIS:HE1	1.58	0.52
1:A:13:GLY:H	1:A:355:HIS:CE1	2.26	0.52
1:A:13:GLY:H	1:A:355:HIS:HE1	1.58	0.52
1:D:278:THR:O	1:D:282:THR:HG23	2.09	0.52
1:D:123:MET:HA	1:D:123:MET:CE	2.32	0.52
1:B:251:THR:HB	1:B:257:VAL:CG2	2.34	0.51
1:C:123:MET:HA	1:C:123:MET:CE	2.33	0.51
1:A:73:ARG:NH1	1:A:75:GLU:OE2	2.44	0.51
1:C:73:ARG:NH1	1:C:75:GLU:OE2	2.44	0.50
1:A:251:THR:HB	1:A:257:VAL:CG2	2.33	0.50
1:A:224:CYS:HA	1:A:324:PHE:CE1	2.45	0.50
1:A:21:MET:CE	1:A:31:THR:HG22	2.41	0.50
1:B:37:LEU:HD22	1:B:37:LEU:C	2.36	0.50
1:B:39:MET:CE	1:B:295:GLY:HA2	2.41	0.49
1:C:378:ARG:O	1:C:379:PHE:C	2.52	0.49
1:B:37:LEU:CD1	1:B:255:GLY:HA3	2.32	0.49
1:B:278:THR:O	1:B:282:THR:HG23	2.12	0.49
1:C:278:THR:O	1:C:282:THR:HG23	2.12	0.48
1:B:224:CYS:HA	1:B:324:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:THR:O	1:A:282:THR:HG23	2.13	0.48
1:C:123:MET:HE2	1:D:123:MET:HB3	1.94	0.48
1:A:123:MET:HA	1:A:123:MET:CE	2.32	0.48
1:C:230:GLU:OE1	3:C:501:HOH:O	2.20	0.47
1:B:37:LEU:C	1:B:37:LEU:CD2	2.82	0.47
1:A:206:PRO:HA	1:B:87:PHE:CE2	2.49	0.47
1:A:213:SER:HB2	3:A:587:HOH:O	2.14	0.47
1:C:394:ILE:O	1:C:397:SER:HB3	2.15	0.47
1:A:21:MET:HE1	1:A:31:THR:HG22	1.97	0.47
1:D:224:CYS:HA	1:D:324:PHE:CE1	2.50	0.46
1:C:251:THR:HB	1:C:257:VAL:CG2	2.34	0.46
1:B:37:LEU:HA	1:B:37:LEU:HD23	1.25	0.46
1:C:87:PHE:CE2	1:D:206:PRO:HA	2.51	0.46
1:C:272:LYS:HD2	3:C:572:HOH:O	2.16	0.46
1:B:285:LYS:N	1:B:286:PRO:CD	2.80	0.45
1:B:395:MET:HE3	1:B:395:MET:HA	1.98	0.45
1:A:368:GLU:O	1:A:372:LYS:HG3	2.16	0.45
1:C:224:CYS:HA	1:C:324:PHE:CE1	2.50	0.45
1:B:395:MET:HA	1:B:395:MET:CE	2.47	0.45
1:C:398:THR:HG21	1:C:400:GLU:OE2	2.17	0.45
1:C:20:VAL:HG13	1:C:166:PRO:HB2	1.99	0.45
1:A:270:LYS:O	1:D:415:LYS:NZ	2.49	0.45
1:D:251:THR:HB	1:D:257:VAL:CG2	2.35	0.45
1:A:20:VAL:HG13	1:A:166:PRO:HB2	1.99	0.45
1:B:398:THR:HG21	1:B:400:GLU:OE2	2.17	0.45
1:C:203:ARG:HB3	1:D:87:PHE:HB2	1.99	0.45
1:A:395:MET:HE3	1:A:395:MET:HA	1.99	0.45
1:D:395:MET:HA	1:D:395:MET:HE3	1.98	0.44
1:D:398:THR:HG21	1:D:400:GLU:OE2	2.17	0.44
1:A:212:ASP:OD2	1:A:214:ASP:HB2	2.17	0.44
1:C:33:ARG:O	1:C:37:LEU:CD2	2.66	0.44
1:C:212:ASP:OD2	1:C:214:ASP:HB2	2.17	0.44
1:D:329:GLY:N	1:D:330:CYS:HA	2.31	0.44
1:B:394:ILE:O	1:B:397:SER:HB3	2.18	0.44
1:C:4:ALA:C	1:C:181:PRO:HG3	2.43	0.43
1:C:79:THR:HG23	1:C:92:SER:OG	2.18	0.43
1:C:395:MET:HA	1:C:395:MET:HE3	1.99	0.43
1:D:20:VAL:HG13	1:D:166:PRO:HB2	2.00	0.43
1:C:285:LYS:N	1:C:286:PRO:CD	2.81	0.43
1:D:394:ILE:O	1:D:397:SER:HB3	2.18	0.43
1:D:395:MET:HA	1:D:395:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:MET:HA	1:A:395:MET:CE	2.49	0.43
1:B:329:GLY:N	1:B:330:CYS:HA	2.34	0.43
1:C:396:GLN:CD	1:C:396:GLN:H	2.26	0.43
1:D:396:GLN:H	1:D:396:GLN:CD	2.27	0.43
1:B:79:THR:HG23	1:B:92:SER:OG	2.19	0.43
1:D:285:LYS:N	1:D:286:PRO:CD	2.81	0.43
1:A:394:ILE:O	1:A:397:SER:HB3	2.18	0.42
1:A:396:GLN:H	1:A:396:GLN:CD	2.27	0.42
1:C:34:PHE:CZ	1:C:166:PRO:HG3	2.54	0.42
1:C:79:THR:CG2	1:C:92:SER:OG	2.68	0.42
1:B:20:VAL:CG1	1:B:40:LYS:CA	2.98	0.42
1:C:395:MET:HA	1:C:395:MET:CE	2.49	0.42
1:A:4:ALA:C	1:A:181:PRO:HG3	2.44	0.42
1:A:213:SER:CB	3:A:587:HOH:O	2.68	0.42
1:B:225:GLU:HB2	1:B:264:MET:HE1	2.01	0.42
1:A:87:PHE:CE2	1:B:206:PRO:HA	2.55	0.42
1:A:123:MET:HE2	1:B:123:MET:HB3	2.01	0.42
1:B:173:VAL:HG11	1:B:303:PHE:HB3	2.02	0.42
1:D:79:THR:HG23	1:D:92:SER:OG	2.21	0.41
1:A:27:ARG:HD2	1:A:165:GLU:OE1	2.20	0.41
1:A:79:THR:HG23	1:A:92:SER:OG	2.20	0.41
1:D:63:ILE:HG22	3:D:673:HOH:O	2.21	0.41
1:A:123:MET:HB3	1:B:123:MET:HE2	2.01	0.41
1:D:35:GLU:C	1:D:37:LEU:H	2.29	0.41
1:C:27:ARG:HD2	1:C:165:GLU:OE1	2.21	0.41
1:D:212:ASP:OD2	1:D:214:ASP:HB2	2.20	0.41
1:B:23:LEU:HG	3:B:677:HOH:O	2.20	0.41
1:C:90:SER:H	1:D:112:GLN:NE2	2.19	0.41
1:C:123:MET:HB3	1:D:123:MET:HE2	2.02	0.41
1:B:79:THR:CG2	1:B:92:SER:OG	2.69	0.41
1:B:212:ASP:OD2	1:B:214:ASP:HB2	2.21	0.41
1:C:113:ALA:N	1:D:88:GLY:O	2.54	0.41
1:C:29:LEU:HD23	1:C:34:PHE:HE2	1.86	0.40
1:C:225:GLU:HB2	1:C:264:MET:HE1	2.03	0.40
1:D:27:ARG:HD2	1:D:165:GLU:OE1	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	403/420 (96%)	379 (94%)	24 (6%)	0	100	100
1	B	396/420 (94%)	371 (94%)	24 (6%)	1 (0%)	36	53
1	C	403/420 (96%)	380 (94%)	23 (6%)	0	100	100
1	D	396/420 (94%)	372 (94%)	24 (6%)	0	100	100
All	All	1598/1680 (95%)	1502 (94%)	95 (6%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	ASN

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	334/348 (96%)	310 (93%)	24 (7%)	13	26
1	B	325/348 (93%)	300 (92%)	25 (8%)	12	23
1	C	336/348 (97%)	313 (93%)	23 (7%)	14	28
1	D	327/348 (94%)	305 (93%)	22 (7%)	15	29
All	All	1322/1392 (95%)	1228 (93%)	94 (7%)	13	26

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	31	THR
1	A	33	ARG
1	A	37	LEU
1	A	53	THR
1	A	60	LYS
1	A	79	THR
1	A	112	GLN
1	A	183	VAL
1	A	198	VAL
1	A	212	ASP
1	A	215	LEU
1	A	217	LEU
1	A	251	THR
1	A	267	LYS
1	A	282	THR
1	A	294	VAL
1	A	316	ASP
1	A	339	THR
1	A	346	ARG
1	A	355	HIS
1	A	395	MET
1	A	397	SER
1	A	408	GLU
1	B	2	VAL
1	B	20	VAL
1	B	21	MET
1	B	27	ARG
1	B	37	LEU
1	B	38	LEU
1	B	53	THR
1	B	60	LYS
1	B	79	THR
1	B	112	GLN
1	B	183	VAL
1	B	198	VAL
1	B	215	LEU
1	B	217	LEU
1	B	251	THR
1	B	267	LYS
1	B	282	THR
1	B	294	VAL
1	B	316	ASP

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Mol	Chain	Res	Type
1	B	339	THR
1	B	346	ARG
1	B	355	HIS
1	B	395	MET
1	B	397	SER
1	B	408	GLU
1	C	27	ARG
1	C	31	THR
1	C	37	LEU
1	C	53	THR
1	C	60	LYS
1	C	79	THR
1	C	112	GLN
1	C	183	VAL
1	C	198	VAL
1	C	212	ASP
1	C	215	LEU
1	C	217	LEU
1	C	251	THR
1	C	267	LYS
1	C	282	THR
1	C	294	VAL
1	C	316	ASP
1	C	339	THR
1	C	346	ARG
1	C	355	HIS
1	C	395	MET
1	C	397	SER
1	C	408	GLU
1	D	27	ARG
1	D	36	ASN
1	D	53	THR
1	D	60	LYS
1	D	79	THR
1	D	112	GLN
1	D	183	VAL
1	D	198	VAL
1	D	212	ASP
1	D	215	LEU
1	D	217	LEU
1	D	251	THR
1	D	267	LYS

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Mol	Chain	Res	Type
1	D	282	THR
1	D	294	VAL
1	D	316	ASP
1	D	339	THR
1	D	346	ARG
1	D	355	HIS
1	D	395	MET
1	D	397	SER
1	D	408	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	112	GLN
1	A	180	ASN
1	A	191	ASN
1	A	344	GLN
1	A	355	HIS
1	B	112	GLN
1	B	342	GLN
1	B	344	GLN
1	B	355	HIS
1	C	112	GLN
1	C	342	GLN
1	C	355	HIS
1	D	104	ASN
1	D	112	GLN
1	D	355	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	PEG	B	501	-	6,6,6	0.59	0	5,5,5	0.41	0
2	PEG	D	502	-	6,6,6	0.90	0	5,5,5	1.05	1 (20%)
2	PEG	D	501	-	6,6,6	0.58	0	5,5,5	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	B	501	-	-	3/4/4/4	-
2	PEG	D	502	-	-	4/4/4/4	-
2	PEG	D	501	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	PEG	C3-O2-C2	2.13	122.58	113.26

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	PEG	O1-C1-C2-O2
2	D	502	PEG	O1-C1-C2-O2
2	B	501	PEG	O1-C1-C2-O2
2	D	502	PEG	O2-C3-C4-O4
2	D	501	PEG	C4-C3-O2-C2
2	D	502	PEG	C1-C2-O2-C3
2	B	501	PEG	C1-C2-O2-C3
2	D	502	PEG	C4-C3-O2-C2
2	D	501	PEG	C1-C2-O2-C3
2	B	501	PEG	O2-C3-C4-O4
2	D	501	PEG	O2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	PEG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	407/420 (96%)	0.45	27 (6%) 24 21	15, 26, 58, 93	0
1	B	402/420 (95%)	0.70	54 (13%) 7 5	15, 27, 71, 104	0
1	C	407/420 (96%)	0.52	37 (9%) 15 13	15, 28, 69, 109	0
1	D	402/420 (95%)	0.58	44 (10%) 10 8	15, 27, 71, 106	0
All	All	1618/1680 (96%)	0.56	162 (10%) 12 10	15, 27, 69, 109	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	161	TRP	7.2
1	A	161	TRP	6.4
1	A	148	PHE	6.2
1	B	148	PHE	6.2
1	B	163	TYR	5.6
1	B	164	ALA	5.6
1	D	30	ASP	5.3
1	D	148	PHE	5.2
1	D	162	SER	5.2
1	B	162	SER	4.9
1	D	213	SER	4.7
1	D	211	GLY	4.7
1	B	20	VAL	4.5
1	C	34	PHE	4.4
1	D	28	HIS	4.4
1	C	396	GLN	4.4
1	B	23	LEU	4.4
1	B	370	LEU	4.4
1	B	34	PHE	4.3
1	D	210	ALA	4.3
1	B	398	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	212	ASP	4.0
1	B	369	LEU	4.0
1	D	398	THR	3.9
1	D	163	TYR	3.9
1	C	148	PHE	3.9
1	B	21	MET	3.9
1	D	291	CYS	3.9
1	B	26	TYR	3.9
1	D	164	ALA	3.9
1	D	376	MET	3.8
1	B	367	TYR	3.8
1	D	35	GLU	3.8
1	D	212	ASP	3.7
1	D	202	CYS	3.7
1	A	398	THR	3.6
1	A	399	GLN	3.6
1	D	215	LEU	3.6
1	B	33	ARG	3.6
1	B	36	ASN	3.6
1	B	35	GLU	3.6
1	D	400	GLU	3.5
1	B	376	MET	3.5
1	D	209	GLU	3.5
1	B	399	GLN	3.5
1	B	273	THR	3.4
1	D	377	VAL	3.4
1	B	396	GLN	3.4
1	A	210	ALA	3.4
1	C	400	GLU	3.4
1	C	163	TYR	3.3
1	B	1	MET	3.3
1	D	39	MET	3.3
1	B	37	LEU	3.3
1	A	35	GLU	3.3
1	B	24	ALA	3.2
1	B	27	ARG	3.2
1	A	396	GLN	3.2
1	B	208	SER	3.1
1	C	211	GLY	3.1
1	D	201	THR	3.1
1	B	397	SER	3.0
1	B	209	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	213	SER	3.0
1	C	377	VAL	3.0
1	C	369	LEU	3.0
1	A	211	GLY	3.0
1	B	167	SER	3.0
1	B	368	GLU	2.9
1	B	377	VAL	2.9
1	D	365	GLU	2.9
1	C	31	THR	2.9
1	D	200	ASP	2.9
1	A	377	VAL	2.9
1	C	367	TYR	2.9
1	B	371	PHE	2.9
1	B	165	GLU	2.9
1	D	208	SER	2.8
1	A	354	LYS	2.8
1	D	23	LEU	2.8
1	D	395	MET	2.8
1	A	214	ASP	2.8
1	C	33	ARG	2.8
1	D	26	TYR	2.7
1	A	207	ASP	2.7
1	D	397	SER	2.7
1	B	210	ALA	2.7
1	C	401	LYS	2.7
1	D	24	ALA	2.7
1	A	397	SER	2.7
1	D	214	ASP	2.7
1	B	200	ASP	2.6
1	A	395	MET	2.6
1	B	211	GLY	2.6
1	B	147	ARG	2.6
1	C	398	THR	2.6
1	B	395	MET	2.6
1	B	213	SER	2.6
1	C	397	SER	2.6
1	C	378	ARG	2.5
1	C	206	PRO	2.5
1	D	394	ILE	2.5
1	C	38	LEU	2.5
1	C	32	ALA	2.5
1	B	207	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	162	SER	2.5
1	A	209	GLU	2.4
1	A	40	LYS	2.4
1	C	391	ILE	2.4
1	D	40	LYS	2.4
1	D	207	ASP	2.4
1	B	214	ASP	2.4
1	B	394	ILE	2.4
1	C	390	MET	2.4
1	B	166	PRO	2.4
1	B	365	GLU	2.4
1	A	212	ASP	2.4
1	C	28	HIS	2.4
1	C	371	PHE	2.4
1	C	35	GLU	2.4
1	D	166	PRO	2.3
1	D	206	PRO	2.3
1	C	395	MET	2.3
1	B	403	ARG	2.3
1	B	215	LEU	2.3
1	C	209	GLU	2.3
1	B	201	THR	2.3
1	B	291	CYS	2.3
1	B	113	ALA	2.3
1	B	393	GLY	2.3
1	C	205	ILE	2.3
1	D	396	GLN	2.2
1	A	208	SER	2.2
1	C	29	LEU	2.2
1	A	400	GLU	2.2
1	C	236	PRO	2.2
1	D	20	VAL	2.2
1	B	372	LYS	2.2
1	B	2	VAL	2.2
1	D	2	VAL	2.2
1	B	212	ASP	2.2
1	A	358	ARG	2.2
1	C	358	ARG	2.2
1	A	215	LEU	2.2
1	D	27	ARG	2.2
1	B	206	PRO	2.2
1	B	275	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	165	GLU	2.1
1	D	102	ASN	2.1
1	C	215	LEU	2.1
1	D	401	LYS	2.1
1	A	391	ILE	2.1
1	A	394	ILE	2.1
1	D	205	ILE	2.1
1	C	399	GLN	2.0
1	A	403	ARG	2.0
1	C	210	ALA	2.0
1	D	370	LEU	2.0
1	C	354	LYS	2.0
1	A	251	THR	2.0
1	A	206	PRO	2.0
1	C	208	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEG	D	502	7/7	0.73	0.17	39,41,43,45	0
2	PEG	B	501	7/7	0.84	0.12	33,34,36,37	0
2	PEG	D	501	7/7	0.85	0.14	29,30,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.