



# Full wwPDB X-ray Structure Validation Report i

Jun 16, 2024 – 03:30 PM EDT

PDB ID : 4YXQ  
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](mailto: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>.

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The following versions of software and data (see [references](#) i) 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 : 2.37.1  
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) : 2.37.1

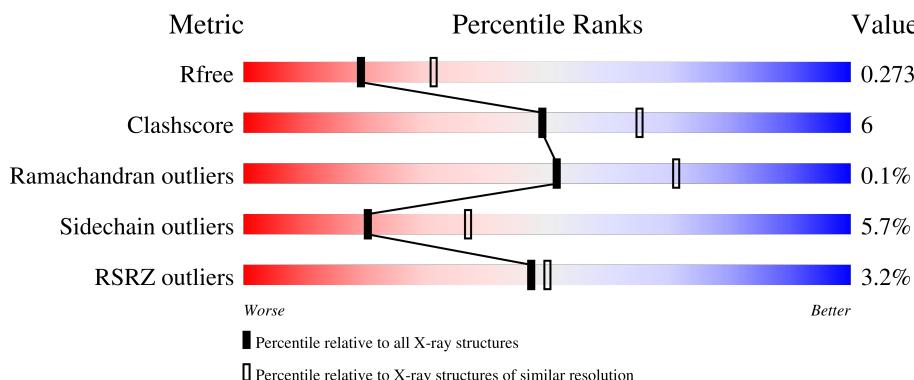
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

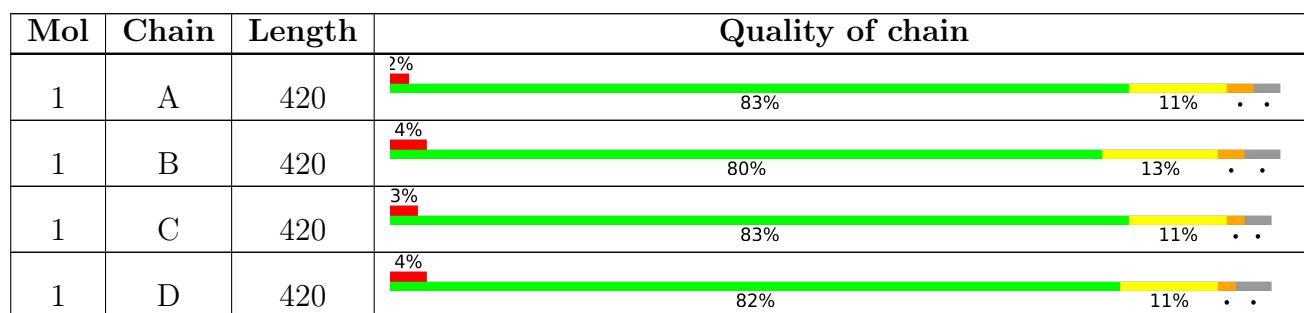
The reported resolution of this entry is 2.47 Å.

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 <sub>free</sub>	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (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 <=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.



## 2 Entry composition [\(i\)](#)

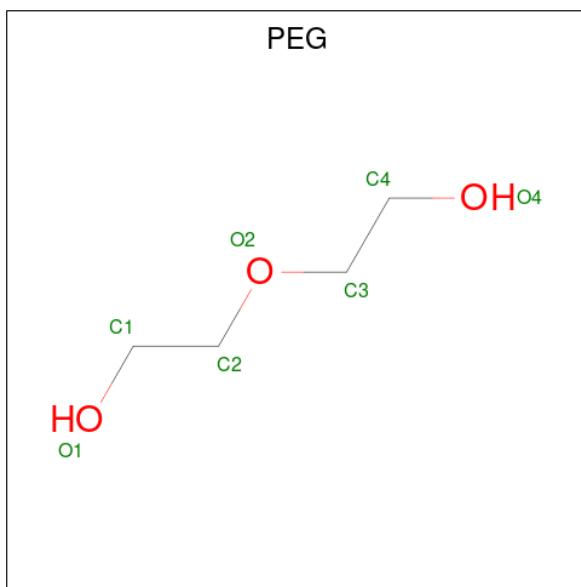
There are 3 unique types of molecules in this entry. The entry contains 12938 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3170	N 2014	O 533	S 599	24	0	0
1	B	402	Total	C 3102	N 1966	O 521	S 590	25	0	0
1	C	407	Total	C 3178	N 2018	O 534	S 602	24	0	0
1	D	402	Total	C 3110	N 1971	O 525	S 590	24	0	0

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

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

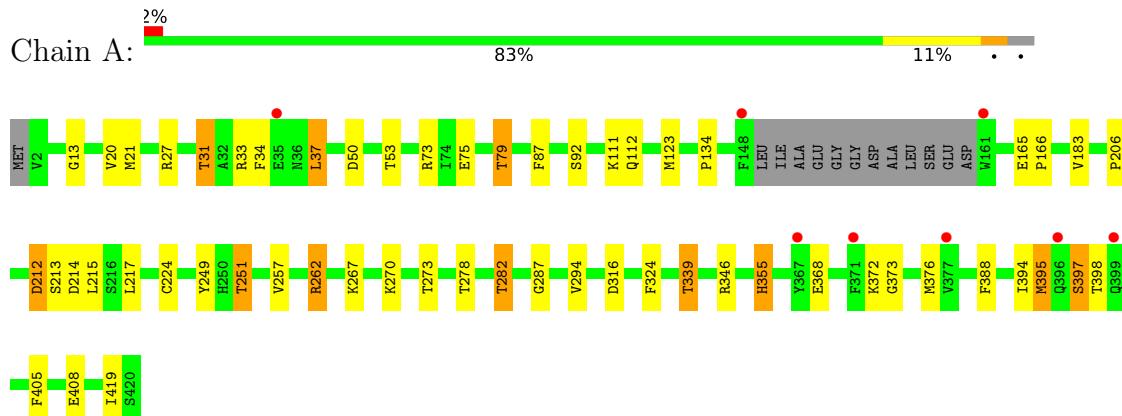
- Molecule 3 is water.

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

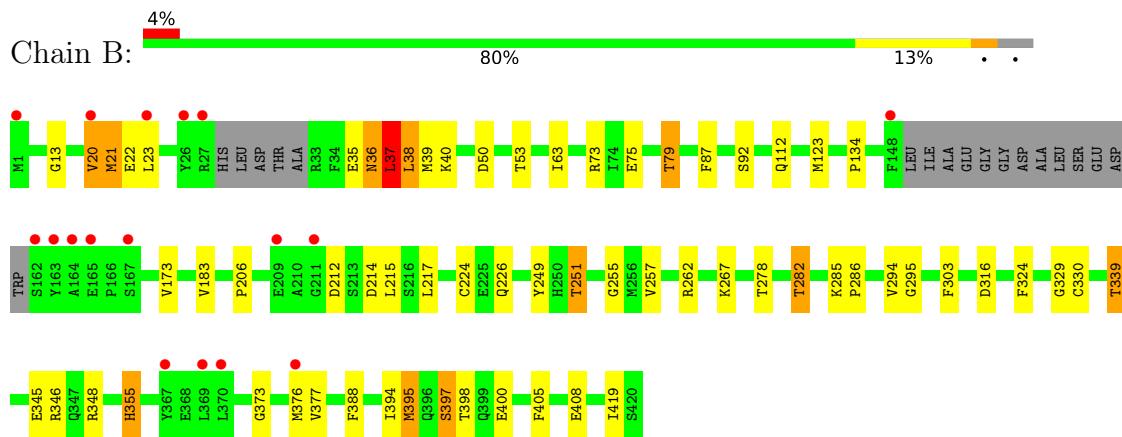
### 3 Residue-property plots

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.

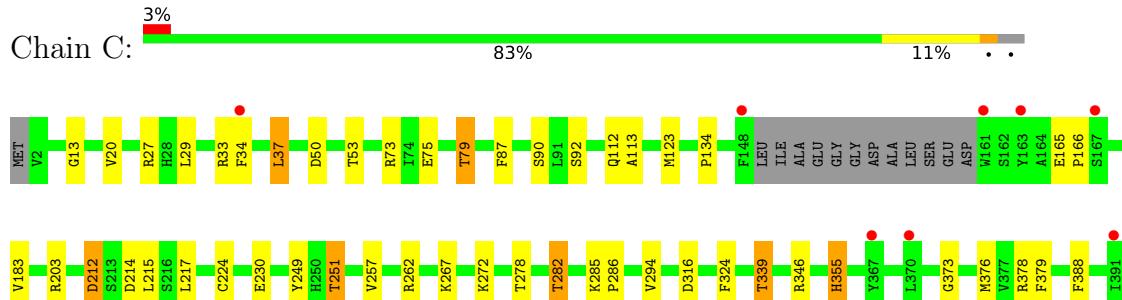
- Molecule 1: Polyketide biosynthesis 3-hydroxy-3-methylglutaryl-ACP synthase PksG



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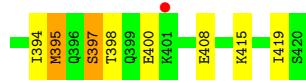
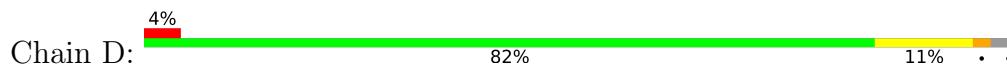


- Molecule 1: Polyketide biosynthesis 3-hydroxy-3-methylglutaryl-ACP synthase PksG





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



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.62 Å   122.04 Å   198.33 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	63.74 – 2.47 63.66 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.74-2.47) 99.9 (63.66-2.47)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.10 (at 2.48 Å)	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 (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 32.5	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49$ , $< L^2 > = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.60	0/3238	0.74	0/4370
1	B	0.62	0/3164	0.77	1/4268 (0.0%)
1	C	0.60	0/3246	0.74	0/4380
1	D	0.65	1/3172 (0.0%)	0.76	0/4277
All	All	0.62	1/12820 (0.0%)	0.75	1/17295 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	343	GLY	C-N	9.68	1.56	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	LEU	CA-CB-CG	-6.17	101.10	115.30

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	A	3170	0	3088	35	0
1	B	3102	0	3013	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3178	0	3098	37	0
1	D	3110	0	3031	34	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	147	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 6.

All (147) 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: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:A:398:THR:HG23	3:A:573:HOH:O	1.68	0.92
1:B:20:VAL:HG12	1:B:40:LYS:C	1.89	0.92
1:C:251:THR:HB	1:C:257:VAL:HG21	1.51	0.91
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: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: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:35:GLU:O	1:B:36:ASN:C	2.22	0.76
1:B:20:VAL:CG1	1:B:40:LYS:C	2.56	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:123:MET:HA	1:D:123:MET:CE	2.32	0.60
1:A:123:MET:HA	1:A:123:MET:CE	2.32	0.59
1:B:183:VAL:O	1:B:339:THR:HB	2.03	0.59
1:C:123:MET:HA	1:C:123:MET:CE	2.33	0.59
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:B:123:MET:HA	1:B:123:MET:CE	2.35	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:251:THR:HB	1:B:257:VAL:CG2	2.34	0.51
1:D:123:MET:HA	1:D:123:MET:HE3	1.92	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:39:MET:CE	1:B:295:GLY:HA2	2.41	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
1:A:278:THR:O	1:A:282:THR:HG23	2.13	0.48
1:C:230:GLU:OE1	3:C:501:HOH:O	2.20	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:395:MET:HE1	1:A:405:PHE:CE2	2.49	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:B:37:LEU:HD22	1:B:37:LEU:C	2.36	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:A:21:MET:HE1	1:A:31:THR:HG22	1.97	0.45
1:B:285:LYS:N	1:B:286:PRO:CD	2.80	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:C:378:ARG:O	1:C:379:PHE:C	2.52	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:B:395:MET:HE1	1:B:405:PHE:CE2	2.52	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:79:THR:HG23	1:C:92:SER:OG	2.18	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:CE	1:D:395:MET:HA	2.48	0.43
1:A:395:MET:CE	1:A:395:MET:HA	2.49	0.43
1:B:39:MET:HE1	1:B:295:GLY:HA2	1.99	0.43
1:B:329:GLY:N	1:B:330:CYS:HA	2.34	0.43
1:B:37:LEU:C	1:B:37:LEU:CD2	2.82	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:C:34:PHE:CZ	1:C:166:PRO:HG3	2.54	0.42
1:B:35:GLU:O	1:B:36:ASN:O	2.37	0.42
1:C:79:THR:CG2	1:C:92:SER:OG	2.68	0.42
1:C:395:MET:HA	1:C:395:MET:HE2	2.02	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:213:SER:CB	3:A:587:HOH:O	2.68	0.42
1:A:87:PHE:CE2	1:B:206:PRO:HA	2.55	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: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: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:D:395:MET:HA	1:D:395:MET:HE2	2.03	0.41
1:A:270:LYS:O	1:D:415:LYS:NZ	2.49	0.40
1:C:29:LEU:HD23	1:C:34:PHE:HE2	1.86	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 [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	403/420 (96%)	379 (94%)	24 (6%)	0	100 100
1	B	396/420 (94%)	371 (94%)	24 (6%)	1 (0%)	41 59
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%)	51 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	ASN

### 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.

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%)	314 (94%)	20 (6%)	19 34
1	B	325/348 (93%)	305 (94%)	20 (6%)	18 33
1	C	336/348 (97%)	318 (95%)	18 (5%)	22 40
1	D	327/348 (94%)	309 (94%)	18 (6%)	21 39
All	All	1322/1392 (95%)	1246 (94%)	76 (6%)	20 37

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	33	ARG
1	A	37	LEU
1	A	79	THR
1	A	112	GLN
1	A	212	ASP
1	A	215	LEU
1	A	217	LEU
1	A	251	THR
1	A	262	ARG
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	20	VAL
1	B	21	MET
1	B	37	LEU
1	B	38	LEU
1	B	79	THR
1	B	112	GLN
1	B	215	LEU
1	B	217	LEU
1	B	251	THR
1	B	262	ARG
1	B	267	LYS
1	B	282	THR
1	B	294	VAL
1	B	316	ASP
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	37	LEU
1	C	79	THR
1	C	112	GLN

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Mol	Chain	Res	Type
1	C	212	ASP
1	C	215	LEU
1	C	217	LEU
1	C	251	THR
1	C	262	ARG
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	36	ASN
1	D	79	THR
1	D	112	GLN
1	D	212	ASP
1	D	215	LEU
1	D	217	LEU
1	D	251	THR
1	D	262	ARG
1	D	267	LYS
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 (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	131	GLN
1	A	191	ASN
1	A	241	GLN
1	A	342	GLN

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Mol	Chain	Res	Type
1	A	355	HIS
1	B	112	GLN
1	B	131	GLN
1	B	241	GLN
1	B	342	GLN
1	B	355	HIS
1	C	112	GLN
1	C	131	GLN
1	C	191	ASN
1	C	241	GLN
1	C	312	GLN
1	C	342	GLN
1	C	355	HIS
1	D	112	GLN
1	D	131	GLN
1	D	191	ASN
1	D	241	GLN
1	D	342	GLN
1	D	355	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 [\(i\)](#)

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	0.58	0	5,5,5	0.41	0
2	PEG	D	501	-	6,6,6	0.57	0	5,5,5	0.70	0
2	PEG	D	502	-	6,6,6	0.90	0	5,5,5	1.06	1 (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
2	PEG	B	501	-	-	3/4/4/4	-
2	PEG	D	501	-	-	3/4/4/4	-
2	PEG	D	502	-	-	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( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	502	PEG	C3-O2-C2	2.15	122.58	113.29

There are no chirality outliers.

All (10) 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

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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	407/420 (96%)	-0.07	8 (1%) 65 67	15, 26, 58, 93	0
1	B	402/420 (95%)	0.06	17 (4%) 36 38	15, 27, 71, 104	0
1	C	407/420 (96%)	0.01	11 (2%) 54 56	15, 28, 69, 109	0
1	D	402/420 (95%)	-0.01	15 (3%) 41 44	15, 27, 71, 106	0
All	All	1618/1680 (96%)	-0.00	51 (3%) 47 50	15, 27, 69, 109	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	PHE	5.7
1	C	161	TRP	5.0
1	D	148	PHE	4.6
1	C	396	GLN	4.4
1	D	162	SER	4.1
1	B	162	SER	3.9
1	D	376	MET	3.8
1	C	34	PHE	3.6
1	A	161	TRP	3.5
1	B	164	ALA	3.4
1	B	370	LEU	3.3
1	D	210	ALA	3.3
1	C	399	GLN	3.2
1	B	20	VAL	3.1
1	A	148	PHE	3.1
1	B	27	ARG	2.9
1	D	212	ASP	2.9
1	B	376	MET	2.9
1	B	163	TYR	2.8
1	D	165	GLU	2.6
1	B	211	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	367	TYR	2.6
1	B	369	LEU	2.6
1	D	211	GLY	2.5
1	D	377	VAL	2.5
1	A	399	GLN	2.5
1	A	367	TYR	2.5
1	A	35	GLU	2.5
1	D	213	SER	2.4
1	B	367	TYR	2.4
1	B	1	MET	2.4
1	D	209	GLU	2.3
1	B	23	LEU	2.3
1	D	215	LEU	2.3
1	C	163	TYR	2.2
1	D	214	ASP	2.2
1	B	167	SER	2.2
1	D	401	LYS	2.1
1	B	209	GLU	2.1
1	C	148	PHE	2.1
1	C	400	GLU	2.1
1	B	26	TYR	2.1
1	D	26	TYR	2.1
1	A	396	GLN	2.1
1	A	371	PHE	2.1
1	C	370	LEU	2.1
1	C	167	SER	2.0
1	C	391	ILE	2.0
1	A	377	VAL	2.0
1	B	165	GLU	2.0
1	D	206	PRO	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PEG	B	501	7/7	0.81	0.20	33,34,36,37	0
2	PEG	D	502	7/7	0.81	0.23	39,41,43,45	0
2	PEG	D	501	7/7	0.88	0.18	29,30,31,32	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.