



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:38 am BST

PDB ID : 2WGF  
Title : Crystal structure of Mycobacterium tuberculosis C171Q KasA variant  
Authors : Luckner, S.R.; Kisker, C.  
Deposited on : 2009-04-17  
Resolution : 2.15 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 ⓘ symbol.

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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

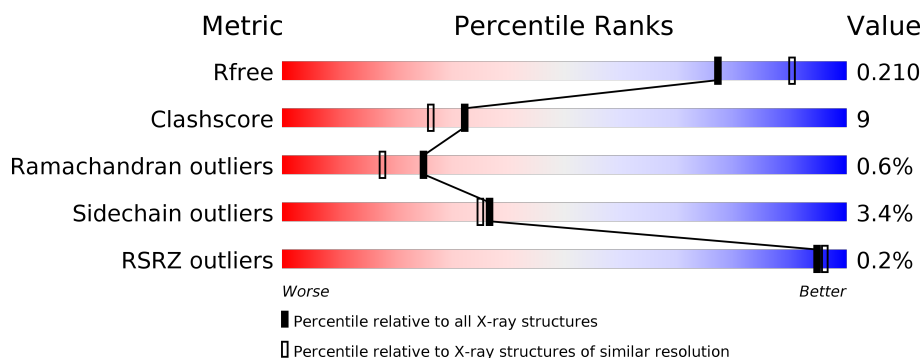
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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  $\geq 3$ , 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	416	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	B	416	<div> <div>79%</div> <div>20%</div> </div>
1	C	416	<div> <div>79%</div> <div>21%</div> </div>
1	D	416	<div> <div>81%</div> <div>18%</div> </div>
1	E	416	<div> <div>77%</div> <div>21%</div> <div>.</div> </div>
1	F	416	<div> <div>74%</div> <div>23%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	416	 75% 23% •
1	H	416	 81% 18% •

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24415 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 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3032	1891	539	585	17			
1	B	415	Total	C	N	O	S	0	1	0
			3038	1895	539	587	17			
1	C	415	Total	C	N	O	S	0	0	0
			3032	1891	539	585	17			
1	D	415	Total	C	N	O	S	0	1	0
			3038	1895	539	587	17			
1	E	415	Total	C	N	O	S	0	0	0
			3032	1891	539	585	17			
1	F	415	Total	C	N	O	S	0	0	0
			3032	1891	539	585	17			
1	G	415	Total	C	N	O	S	0	0	0
			3032	1891	539	585	17			
1	H	415	Total	C	N	O	S	0	1	0
			3038	1895	539	587	17			

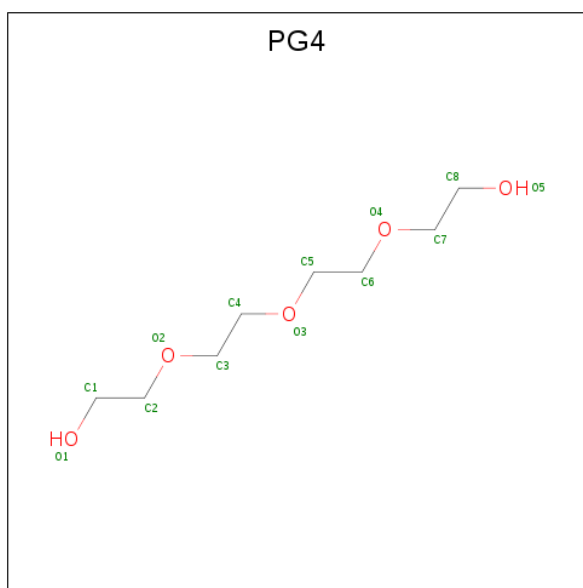
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLN	CYS	engineered mutation	UNP P63454
B	171	GLN	CYS	engineered mutation	UNP P63454
C	171	GLN	CYS	engineered mutation	UNP P63454
D	171	GLN	CYS	engineered mutation	UNP P63454
E	171	GLN	CYS	engineered mutation	UNP P63454
F	171	GLN	CYS	engineered mutation	UNP P63454
G	171	GLN	CYS	engineered mutation	UNP P63454
H	171	GLN	CYS	engineered mutation	UNP P63454

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



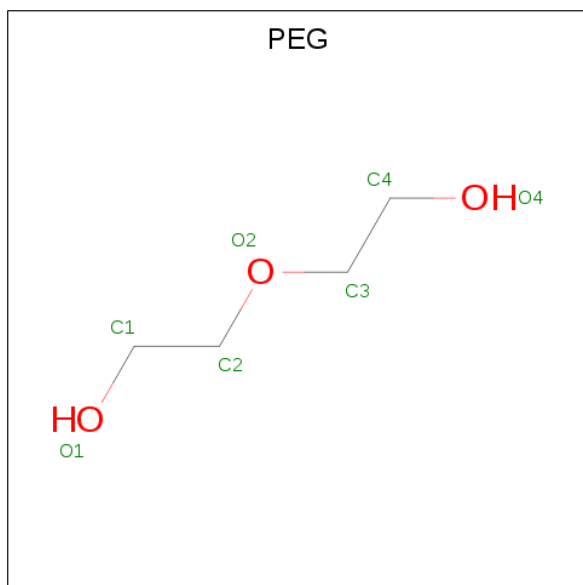
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 13 8 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			13	8	5		
3	E	1	Total	C	O	0	0
			13	8	5		
3	F	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 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
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

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

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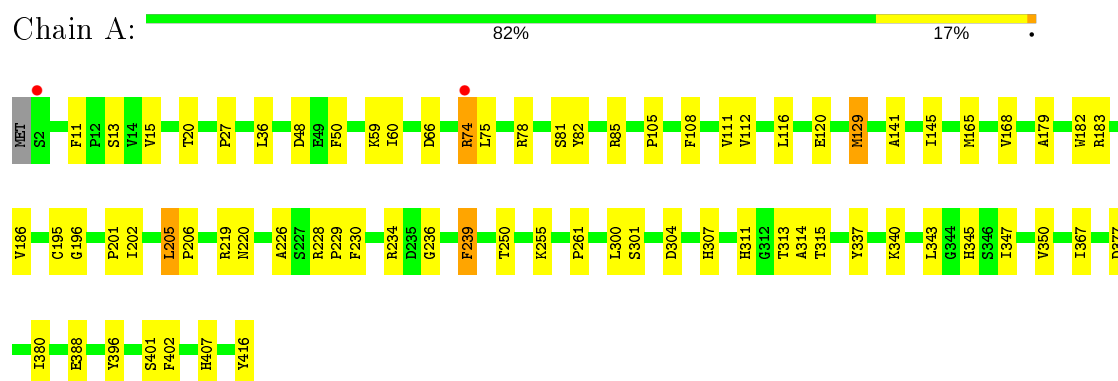
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	4	Total	O	0	0
			4	4		
5	G	3	Total	O	0	0
			3	3		
5	H	5	Total	O	0	0
			5	5		

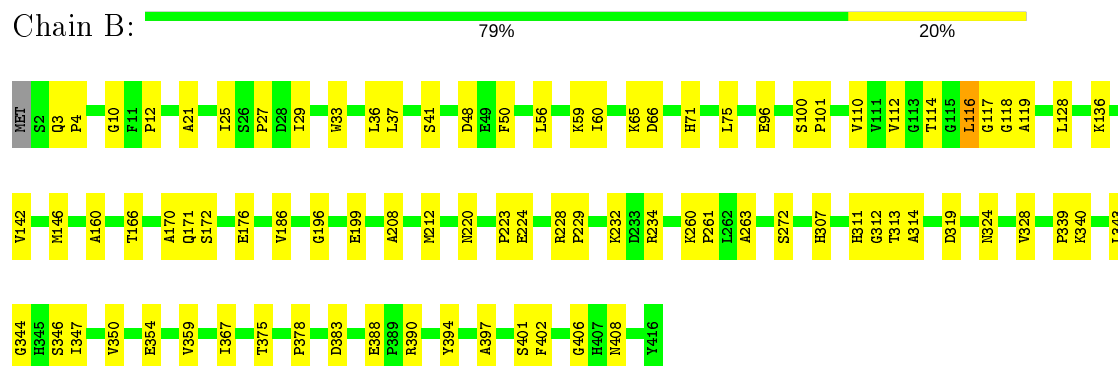
### 3 Residue-property plots

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

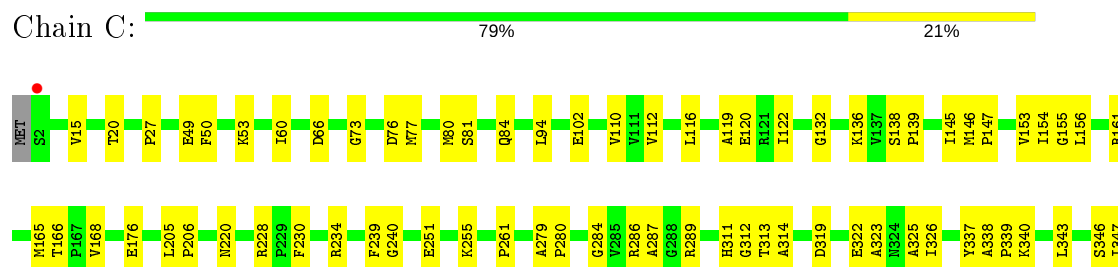
#### • Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1



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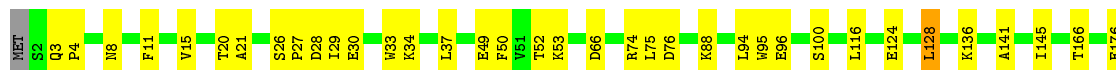






• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1

Chain D: 81% 18%



• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1

Chain E: 77% 21%



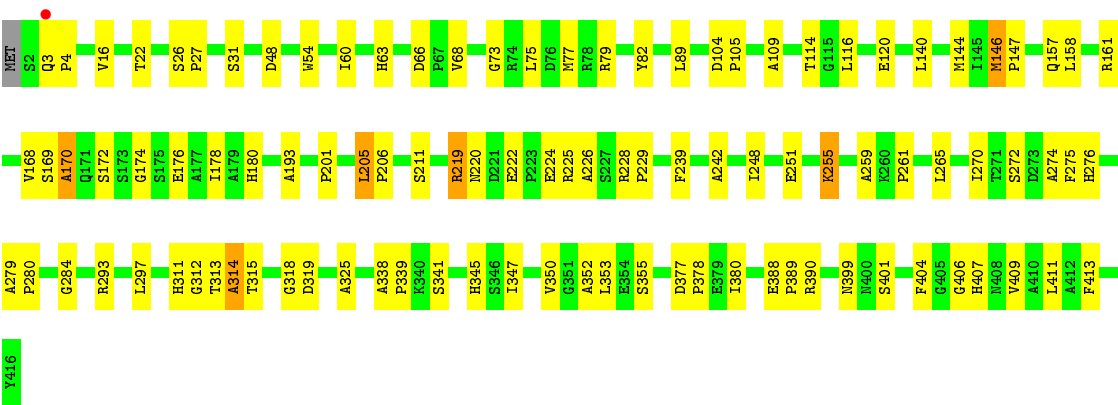
• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1

Chain F: 74% 23%

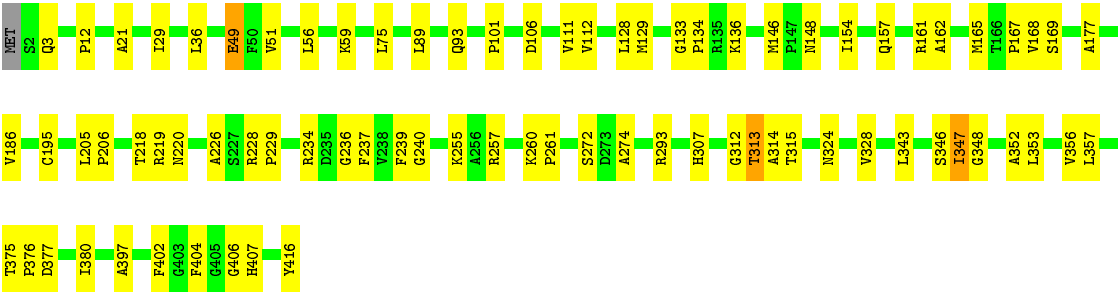
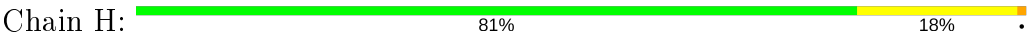


• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1

Chain G: 75% 23%



● Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.50Å 151.50Å 147.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.71 – 2.15 33.71 – 2.15	Depositor EDS
% Data completeness (in resolution range)	67.9 (33.71-2.15) 92.3 (33.71-2.15)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.16Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.166 , 0.211 0.168 , 0.210	Depositor DCC
$R_{free}$ test set	9673 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 35.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.108 for -h,-k,l 0.437 for h,-h-k,-l 0.108 for -k,-h,-l	Xtriage
Reported twinning fraction	0.452 for h,-h-k,-l	Depositor
Outliers	0 of 190497 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	24415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup> Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PG4, 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	0.30	0/3092	0.47	0/4201
1	B	0.30	0/3101	0.50	0/4214
1	C	0.31	0/3092	0.50	0/4201
1	D	0.32	0/3101	0.51	0/4214
1	E	0.30	0/3092	0.48	0/4201
1	F	0.28	0/3092	0.47	0/4201
1	G	0.28	0/3092	0.47	0/4201
1	H	0.30	0/3101	0.48	0/4214
All	All	0.30	0/24763	0.49	0/33647

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3032	0	2985	42	0
1	B	3038	0	2991	54	0
1	C	3032	0	2985	52	0
1	D	3038	0	2991	45	0
1	E	3032	0	2985	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3032	0	2985	73	0
1	G	3032	0	2985	62	0
1	H	3038	0	2991	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	13	0	18	2	0
3	B	26	0	36	1	0
3	C	13	0	18	1	0
3	D	13	0	18	1	0
3	E	13	0	18	3	0
3	F	13	0	18	1	0
4	D	7	0	10	0	0
5	A	4	0	0	0	0
5	B	3	0	0	1	0
5	C	7	0	0	0	0
5	D	7	0	0	0	0
5	E	2	0	0	0	0
5	F	4	0	0	0	0
5	G	3	0	0	0	0
5	H	5	0	0	0	0
All	All	24415	0	24034	425	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 9.

All (425) 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:339:PRO:HG2	1:B:354:GLU:HG2	1.56	0.87
1:H:237:PHE:HB3	1:H:313:THR:HG23	1.59	0.84
1:C:27:PRO:HG3	1:C:66:ASP:HB2	1.62	0.82
1:G:27:PRO:HG3	1:G:66:ASP:HB2	1.65	0.79
1:H:219:ARG:HD3	1:H:226:ALA:HA	1.65	0.77
1:H:377:ASP:HB3	1:H:380:ILE:CG1	2.14	0.77
1:D:27:PRO:HG3	1:D:66:ASP:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:PRO:HG3	1:C:66:ASP:CB	2.16	0.75
1:H:377:ASP:HB3	1:H:380:ILE:HG13	1.69	0.74
1:B:116:LEU:HG	3:B:1417:PG4:H41	1.69	0.74
1:D:49:GLU:OE1	1:D:49:GLU:HA	1.86	0.74
1:F:157:GLN:HG2	1:F:158:LEU:HD13	1.70	0.74
1:H:51:VAL:HA	1:H:56:LEU:HD12	1.70	0.73
1:F:111:VAL:HG13	1:F:165:MET:HB2	1.71	0.72
1:G:146:MET:HE1	1:H:404:PHE:HB2	1.72	0.70
1:E:234:ARG:HE	1:E:316:PRO:HA	1.55	0.69
1:G:272:SER:HA	1:G:406:GLY:O	1.93	0.69
1:E:27:PRO:HG3	1:E:66:ASP:HB3	1.75	0.69
1:F:232:LYS:HD2	1:F:378:PRO:HD2	1.75	0.69
1:D:343:LEU:HD13	1:D:353:LEU:HD21	1.75	0.68
1:B:116:LEU:HD12	1:B:117:GLY:N	2.09	0.68
1:D:286:ARG:NH2	1:D:289:ARG:HG2	2.09	0.68
1:D:205:LEU:HB3	1:D:206:PRO:HD3	1.76	0.66
1:F:110:VAL:HB	1:F:164:VAL:HG22	1.77	0.65
1:G:147:PRO:HB2	1:H:168:VAL:HG21	1.77	0.65
1:G:226:ALA:O	1:G:228:ARG:HG3	1.96	0.65
1:H:240:GLY:O	1:H:346:SER:HB3	1.97	0.64
1:F:305:ILE:HD12	1:F:398:VAL:HG23	1.80	0.64
1:F:167:PRO:HG3	1:F:177:ALA:HA	1.79	0.64
1:B:118:GLY:HA2	5:B:2001:HOH:O	1.97	0.63
1:C:112:VAL:O	1:C:166:THR:HG23	1.99	0.62
1:H:377:ASP:HB3	1:H:380:ILE:HG12	1.81	0.62
1:H:313:THR:HG22	1:H:315:THR:HG23	1.82	0.61
1:F:272:SER:HA	1:F:406:GLY:O	2.01	0.61
1:F:56:LEU:O	1:F:59:LYS:HE3	2.01	0.60
1:B:311:HIS:CD2	1:B:313:THR:HG23	2.36	0.60
1:D:228:ARG:HG2	1:D:372:ASN:HB3	1.82	0.60
1:F:68:VAL:HG22	1:F:89:LEU:HD23	1.83	0.60
1:E:74:ARG:O	1:E:77:MET:HB2	2.02	0.60
1:G:313:THR:O	1:G:314:ALA:HB3	2.02	0.60
1:H:59:LYS:H	1:H:220:ASN:ND2	2.00	0.60
1:C:205:LEU:HD12	3:C:1417:PG4:H22	1.84	0.59
1:G:377:ASP:HB3	1:G:380:ILE:HG12	1.84	0.59
1:A:236:GLY:HA2	1:A:315:THR:HG22	1.85	0.59
1:E:50:PHE:HB2	1:E:54:TRP:CD1	2.37	0.59
1:B:27:PRO:HG3	1:B:66:ASP:HB2	1.83	0.59
1:H:313:THR:CG2	1:H:315:THR:HG23	2.33	0.59
1:B:229:PRO:HD3	1:B:314:ALA:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ILE:HG13	1:D:360:LEU:HD11	1.84	0.58
1:G:75:LEU:HD22	1:G:79:ARG:HD3	1.85	0.58
1:C:205:LEU:HB3	1:C:206:PRO:HD3	1.85	0.58
1:F:101:PRO:HG3	1:F:257:ARG:NH2	2.19	0.58
1:F:313:THR:O	1:F:314:ALA:HB3	2.03	0.58
1:G:274:ALA:HB3	1:H:161:ARG:HE	1.68	0.58
1:A:27:PRO:HB3	1:A:66:ASP:HB3	1.86	0.58
1:A:111:VAL:O	1:A:195:CYS:HA	2.04	0.58
1:F:157:GLN:HG2	1:F:158:LEU:CD1	2.34	0.58
1:B:36:LEU:HD11	1:B:343:LEU:HD11	1.86	0.58
1:G:265:LEU:HD13	1:G:413:PHE:CE1	2.39	0.58
1:A:377:ASP:HB3	1:A:380:ILE:HD12	1.85	0.57
1:C:73:GLY:O	1:C:77:MET:HG2	2.03	0.57
1:D:327:ARG:HG2	1:D:332:ASP:OD2	2.04	0.57
1:F:260:LYS:HD2	1:F:261:PRO:HD2	1.86	0.57
1:C:112:VAL:HG21	1:C:154:ILE:HD12	1.87	0.57
1:D:286:ARG:HH22	1:D:289:ARG:HG2	1.70	0.57
1:A:261:PRO:HG2	1:A:416:TYR:CE1	2.39	0.57
1:C:287:ALA:HB1	1:C:402:PHE:CE1	2.40	0.57
1:D:15:VAL:HB	1:D:261:PRO:HB3	1.87	0.57
1:H:167:PRO:HG2	1:H:177:ALA:HA	1.87	0.57
1:E:27:PRO:HG3	1:E:66:ASP:CB	2.34	0.56
1:F:264:ARG:HB3	1:F:266:LEU:HD21	1.86	0.56
1:E:207:ILE:O	1:E:211:SER:HB2	2.04	0.56
1:H:21:ALA:HB3	1:H:29:ILE:HD13	1.87	0.56
1:G:275:PHE:CD2	1:G:276:HIS:HB2	2.41	0.56
1:H:106:ASP:O	1:H:162:ALA:HB2	2.06	0.56
1:B:4:PRO:HB3	1:B:10:GLY:HA3	1.88	0.55
1:C:81:SER:OG	1:C:84:GLN:HG3	2.06	0.55
1:D:20:THR:HG21	1:D:94:LEU:HB2	1.89	0.55
1:E:50:PHE:HB2	1:E:54:TRP:HD1	1.72	0.55
1:E:20:THR:HG22	1:E:245:LEU:HB2	1.86	0.55
1:B:59:LYS:H	1:B:220:ASN:ND2	2.04	0.55
1:E:313:THR:O	1:E:314:ALA:HB3	2.06	0.55
1:H:343:LEU:HD13	1:H:353:LEU:HD21	1.88	0.55
1:A:15:VAL:HB	1:A:261:PRO:HB3	1.89	0.55
1:C:377:ASP:OD1	1:C:378:PRO:HD2	2.07	0.55
1:E:100:SER:N	1:E:101:PRO:HD3	2.21	0.55
1:A:311:HIS:CD2	1:A:313:THR:HG23	2.42	0.55
1:C:383:ASP:OD2	1:C:390:ARG:NH1	2.39	0.54
1:F:20:THR:CG2	1:F:94:LEU:HB2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:SER:HA	1:F:401:SER:HB3	1.90	0.54
1:A:168:VAL:HG23	1:B:166:THR:HB	1.89	0.54
1:C:50:PHE:HA	1:C:53:LYS:HB3	1.89	0.54
1:C:102:GLU:OE1	1:C:102:GLU:HA	2.07	0.54
1:C:353:LEU:O	1:C:357:LEU:HG	2.08	0.54
1:H:205:LEU:HB3	1:H:206:PRO:HD3	1.89	0.54
1:A:205:LEU:HB3	1:A:206:PRO:HD3	1.90	0.54
1:B:340:LYS:HG2	1:B:344:GLY:O	2.08	0.54
1:E:36:LEU:HD11	1:E:343:LEU:HD11	1.90	0.54
1:H:12:PRO:HD2	1:H:186:VAL:HG12	1.89	0.54
1:B:41:SER:HB3	1:B:224:GLU:OE2	2.08	0.53
1:E:311:HIS:CD2	1:E:313:THR:HG23	2.43	0.53
1:G:161:ARG:HE	1:H:274:ALA:HB3	1.73	0.53
1:G:259:ALA:O	1:G:261:PRO:HD3	2.09	0.53
1:B:25:ILE:O	1:B:65:LYS:HG2	2.08	0.53
1:B:60:ILE:HG22	1:B:223:PRO:HG3	1.90	0.53
1:H:89:LEU:O	1:H:93:GLN:HG3	2.09	0.53
1:F:313:THR:O	1:F:314:ALA:CB	2.57	0.53
1:H:324:ASN:O	1:H:328:VAL:HG23	2.09	0.53
1:B:12:PRO:HD2	1:B:186:VAL:HB	1.91	0.53
1:G:73:GLY:O	1:G:77:MET:HG2	2.09	0.53
1:G:75:LEU:HD22	1:G:79:ARG:CD	2.39	0.53
1:A:234:ARG:HB2	1:A:314:ALA:O	2.09	0.52
1:F:20:THR:HG21	1:F:94:LEU:HB2	1.90	0.52
1:E:234:ARG:HB2	1:E:314:ALA:O	2.09	0.52
1:A:205:LEU:HD12	3:A:1418:PG4:H21	1.90	0.52
1:C:251:GLU:O	1:C:255:LYS:HB2	2.10	0.52
1:F:205:LEU:HB3	1:F:206:PRO:HD3	1.91	0.52
1:G:205:LEU:HB3	1:G:206:PRO:HD3	1.92	0.52
1:F:19:VAL:HB	1:F:356:VAL:HG13	1.92	0.52
1:F:43:ILE:HG21	1:F:238:VAL:HG11	1.91	0.52
1:D:50:PHE:HA	1:D:53:LYS:HB3	1.92	0.52
1:F:313:THR:HA	1:F:340:LYS:HD2	1.91	0.52
1:G:140:LEU:O	1:G:144:MET:HG3	2.09	0.52
1:F:153:VAL:O	1:F:157:GLN:HB3	2.09	0.52
1:B:383:ASP:CG	1:B:390:ARG:HH22	2.13	0.52
1:G:176:GLU:HG2	1:G:180:HIS:CD2	2.45	0.51
1:C:228:ARG:O	1:C:234:ARG:HB3	2.09	0.51
1:G:27:PRO:HG3	1:G:66:ASP:CB	2.35	0.51
1:F:379:GLU:OE1	1:F:379:GLU:HA	2.10	0.51
1:G:293:ARG:NH2	1:G:297:LEU:HD21	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ALA:O	1:A:183:ARG:HG3	2.10	0.51
1:E:110:VAL:HG23	1:E:160:ALA:CB	2.41	0.51
1:E:130:ASN:HA	1:F:54:TRP:HH2	1.75	0.51
1:D:313:THR:O	1:D:314:ALA:HB3	2.10	0.51
1:C:168:VAL:HG23	1:D:166:THR:HB	1.92	0.51
1:F:113:GLY:O	1:F:197:GLY:HA2	2.11	0.51
1:C:161:ARG:HE	1:D:274:ALA:HB3	1.76	0.51
1:F:339:PRO:HG2	1:F:354:GLU:HG2	1.93	0.51
1:G:157:GLN:HE21	1:G:158:LEU:HG	1.74	0.51
1:H:146:MET:HB2	1:H:148:ASN:OD1	2.11	0.51
1:E:205:LEU:HB3	1:E:206:PRO:HD3	1.92	0.51
1:F:273:ASP:OD1	1:F:286:ARG:HB2	2.11	0.50
1:B:12:PRO:HG2	1:B:186:VAL:HA	1.93	0.50
1:E:232:LYS:HD2	1:E:378:PRO:HD3	1.93	0.50
1:A:337:TYR:HB2	1:A:367:ILE:CG2	2.40	0.50
1:B:228:ARG:O	1:B:234:ARG:HB3	2.11	0.50
1:B:324:ASN:O	1:B:328:VAL:HG23	2.11	0.50
1:C:27:PRO:HG3	1:C:66:ASP:HB3	1.93	0.50
1:G:169:SER:HB2	1:G:407:HIS:CG	2.46	0.50
1:A:228:ARG:O	1:A:234:ARG:HB3	2.12	0.50
1:E:266:LEU:O	1:E:298:ALA:HA	2.11	0.50
1:F:136:LYS:N	1:F:136:LYS:HD3	2.27	0.50
1:B:172:SER:HA	1:B:401:SER:OG	2.11	0.50
1:D:339:PRO:CG	1:D:354:GLU:HG2	2.42	0.50
1:F:110:VAL:O	1:F:164:VAL:HA	2.11	0.50
1:B:388[A]:GLU:HG2	1:C:156:LEU:HD21	1.92	0.50
1:E:187:MET:SD	1:F:183:ARG:HD3	2.52	0.50
1:E:379:GLU:OE1	1:E:379:GLU:HA	2.11	0.49
1:H:111:VAL:HA	1:H:165:MET:O	2.12	0.49
1:F:313:THR:HG22	1:F:340:LYS:HE2	1.93	0.49
1:G:284:GLY:O	1:G:325:ALA:HA	2.12	0.49
1:A:74:ARG:O	1:A:78:ARG:HG3	2.12	0.49
1:C:284:GLY:O	1:C:325:ALA:HA	2.12	0.49
1:D:206:PRO:HA	3:D:1417:PG4:H42	1.95	0.49
1:D:284:GLY:O	1:D:325:ALA:HA	2.12	0.49
1:D:20:THR:HG22	1:D:94:LEU:HD13	1.94	0.49
1:D:219:ARG:HH11	1:D:225:ARG:NH1	2.10	0.49
1:E:167:PRO:HG2	1:E:177:ALA:HA	1.93	0.49
1:H:111:VAL:HG13	1:H:165:MET:HB2	1.94	0.49
1:H:49:GLU:HA	1:H:49:GLU:OE2	2.12	0.49
1:A:337:TYR:HB2	1:A:367:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:HIS:HE1	1:F:337:TYR:HB3	1.77	0.49
1:E:114:THR:HG23	1:E:198:VAL:O	2.13	0.49
1:H:307:HIS:HB3	1:H:397:ALA:HB2	1.95	0.49
1:B:208:ALA:O	1:B:212:MET:HG2	2.13	0.49
1:A:36:LEU:HD11	1:A:343:LEU:HD11	1.95	0.48
1:B:311:HIS:NE2	1:B:313:THR:HG23	2.27	0.48
1:D:30:GLU:O	1:D:34:LYS:HG3	2.14	0.48
1:D:311:HIS:CD2	1:D:313:THR:HG23	2.49	0.48
1:A:313:THR:HG22	1:A:345:HIS:CD2	2.49	0.48
1:E:276:HIS:HB3	1:E:279:ALA:O	2.12	0.48
1:E:199:GLU:HG2	1:E:346:SER:O	2.13	0.48
1:G:270:ILE:HG12	1:G:409:VAL:HG22	1.94	0.48
1:C:165:MET:HG2	1:D:176:GLU:OE2	2.14	0.48
1:C:20:THR:HG21	1:C:94:LEU:HB2	1.95	0.48
1:C:80:MET:CE	1:C:153:VAL:HG11	2.44	0.48
1:C:76:ASP:O	1:C:80:MET:HB2	2.14	0.48
1:E:232:LYS:HD2	1:E:378:PRO:CD	2.44	0.48
1:H:313:THR:O	1:H:314:ALA:HB3	2.14	0.48
1:C:146:MET:HA	1:C:147:PRO:HD3	1.74	0.48
1:G:404:PHE:HB2	1:H:146:MET:HE1	1.96	0.48
1:E:205:LEU:HD12	3:E:1417:PG4:C5	2.44	0.47
1:E:353:LEU:O	1:E:356:VAL:HB	2.13	0.47
1:E:382:LEU:O	1:E:384:VAL:N	2.46	0.47
1:H:353:LEU:O	1:H:357:LEU:HG	2.14	0.47
1:B:313:THR:O	1:B:314:ALA:HB3	2.14	0.47
1:E:56:LEU:O	1:E:59:LYS:NZ	2.43	0.47
1:G:355:SER:OG	1:G:399:ASN:ND2	2.46	0.47
1:G:377:ASP:HA	1:G:378:PRO:HD3	1.76	0.47
1:G:82:TYR:CE1	1:G:201:PRO:HG3	2.49	0.47
1:E:291:MET:O	1:E:295:LEU:HG	2.14	0.47
1:F:108:PHE:HE2	1:F:158:LEU:HB3	1.80	0.47
1:H:111:VAL:O	1:H:195:CYS:HA	2.15	0.47
1:A:129:MET:HE3	1:A:129:MET:HB3	1.89	0.47
1:A:219:ARG:HD2	1:A:226:ALA:HA	1.96	0.47
1:H:352:ALA:O	1:H:356:VAL:HG23	2.14	0.47
1:H:169:SER:HB2	1:H:407:HIS:CG	2.49	0.47
1:A:105:PRO:HA	1:A:108:PHE:HB3	1.97	0.47
1:F:36:LEU:HD11	1:F:343:LEU:HD11	1.97	0.47
1:G:48:ASP:OD2	1:G:63:HIS:NE2	2.37	0.47
1:A:313:THR:O	1:A:314:ALA:HB3	2.15	0.47
3:E:1417:PG4:H82	1:F:142:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:GLY:HA3	1:C:343:LEU:O	2.15	0.47
1:E:63:HIS:CE1	1:E:202:ILE:HB	2.50	0.46
1:F:84:GLN:HB3	1:F:153:VAL:HG11	1.95	0.46
1:H:228:ARG:O	1:H:234:ARG:HB3	2.15	0.46
1:E:227:SER:HB3	1:E:341:SER:HA	1.96	0.46
1:A:340:LYS:HE3	1:A:350:VAL:HG21	1.98	0.46
1:G:109:ALA:O	1:G:193:ALA:HA	2.16	0.46
1:H:261:PRO:HG2	1:H:416:TYR:CE1	2.50	0.46
1:C:60:ILE:HG12	1:C:220:ASN:ND2	2.31	0.46
1:H:112:VAL:HG21	1:H:154:ILE:HD12	1.97	0.46
1:D:208:ALA:O	1:D:212:MET:HG2	2.15	0.46
1:A:205:LEU:HD12	3:A:1418:PG4:C2	2.46	0.46
1:D:377:ASP:HB3	1:D:380:ILE:HG12	1.98	0.46
1:E:236:GLY:HA2	1:E:315:THR:HG22	1.96	0.46
1:F:268:ALA:O	1:F:297:LEU:HD12	2.14	0.46
1:B:100:SER:N	1:B:101:PRO:HD3	2.31	0.46
1:H:101:PRO:HB3	1:H:257:ARG:NH2	2.31	0.46
1:F:36:LEU:HD21	1:F:343:LEU:HG	1.98	0.46
1:G:219:ARG:HD2	1:G:226:ALA:HA	1.98	0.46
1:C:132:GLY:HA3	1:C:136:LYS:HG3	1.97	0.46
1:F:352:ALA:O	1:F:356:VAL:HG23	2.15	0.46
1:H:36:LEU:HD21	1:H:343:LEU:HG	1.98	0.46
1:D:124:GLU:HG2	1:D:128:LEU:HD22	1.97	0.45
1:F:311:HIS:O	1:F:312:GLY:C	2.54	0.45
1:A:402:PHE:HA	1:A:407:HIS:O	2.16	0.45
1:F:225:ARG:HA	1:F:372:ASN:ND2	2.31	0.45
1:F:313:THR:HA	1:F:340:LYS:CD	2.47	0.45
1:C:340:LYS:HE3	1:C:350:VAL:HG21	1.97	0.45
1:G:169:SER:O	1:G:170:ALA:HB3	2.16	0.45
1:G:27:PRO:CG	1:G:66:ASP:HB2	2.41	0.45
1:B:232:LYS:CE	1:B:378:PRO:HD2	2.47	0.45
1:D:33:TRP:O	1:D:37:LEU:HG	2.17	0.45
1:C:240:GLY:O	1:C:346:SER:HB3	2.16	0.45
1:A:182:TRP:O	1:A:186:VAL:HG22	2.16	0.45
1:E:120:GLU:HA	3:E:1417:PG4:H12	1.98	0.45
1:G:16:VAL:HG22	1:G:248:ILE:HG22	1.97	0.45
1:D:76:ASP:OD2	1:D:88:LYS:NZ	2.49	0.45
1:F:42:GLY:O	1:F:44:HIS:HD2	1.99	0.45
1:G:338:ALA:HA	1:G:339:PRO:HD2	1.79	0.45
1:A:165:MET:HG2	1:B:176:GLU:OE2	2.16	0.45
1:A:50:PHE:CD1	1:A:50:PHE:C	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:PHE:CD1	1:C:319:ASP:HB3	2.52	0.45
1:D:141:ALA:O	1:D:145:ILE:HG13	2.17	0.45
1:F:377:ASP:HB3	1:F:380:ILE:HD12	1.99	0.45
1:B:229:PRO:HA	1:B:314:ALA:HA	1.99	0.45
1:B:21:ALA:HB3	1:B:29:ILE:HD13	1.99	0.45
1:B:307:HIS:ND1	1:B:367:ILE:HD13	2.32	0.45
1:E:250:THR:OG1	1:E:253:HIS:HB2	2.17	0.45
1:H:236:GLY:HA2	1:H:315:THR:HG22	1.98	0.45
1:C:322:GLU:O	1:C:326:ILE:HG13	2.17	0.45
1:A:300:LEU:HD11	1:A:396:TYR:CD1	2.52	0.44
1:E:274:ALA:HB3	1:F:161:ARG:HE	1.82	0.44
1:F:35:GLY:O	1:F:40:GLU:HB2	2.16	0.44
1:A:11:PHE:CD1	1:A:186:VAL:HB	2.52	0.44
1:G:311:HIS:CD2	1:G:313:THR:HG23	2.51	0.44
1:B:367:ILE:HG13	1:B:394:TYR:CE2	2.52	0.44
1:G:251:GLU:O	1:G:255:LYS:HB2	2.17	0.44
1:D:239:PHE:HE1	1:D:347:ILE:HD11	1.83	0.44
1:G:313:THR:O	1:G:314:ALA:CB	2.65	0.44
1:G:242:ALA:HB1	1:G:353:LEU:HD22	1.99	0.44
1:C:286:ARG:NH2	1:C:289:ARG:HG2	2.33	0.44
1:F:261:PRO:HG2	1:F:416:TYR:CZ	2.52	0.44
1:A:229:PRO:O	1:A:230:PHE:HB2	2.18	0.44
1:D:339:PRO:HG3	1:D:354:GLU:HG2	1.99	0.44
1:E:369:PRO:HD3	1:E:389:PRO:HD3	1.98	0.44
1:G:315:THR:OG1	1:G:318:GLY:HA3	2.16	0.44
1:E:26:SER:HA	1:E:27:PRO:HD3	1.84	0.44
1:F:205:LEU:HD23	3:F:1417:PG4:H81	1.99	0.44
1:F:264:ARG:NE	1:F:416:TYR:HA	2.33	0.44
1:A:82:TYR:CD2	1:A:201:PRO:HD3	2.53	0.44
1:B:116:LEU:CD1	1:B:119:ALA:HB2	2.48	0.44
1:D:356:VAL:O	1:D:360:LEU:HG	2.16	0.44
1:F:124:GLU:O	1:F:128:LEU:HB2	2.18	0.44
1:A:202:ILE:HG12	1:A:239:PHE:HB3	1.99	0.44
1:C:313:THR:O	1:C:314:ALA:HB3	2.18	0.44
1:G:352:ALA:O	1:G:355:SER:HB2	2.17	0.43
1:G:390:ARG:HE	1:G:390:ARG:HB2	1.66	0.43
1:H:146:MET:HB3	1:H:146:MET:HE3	1.84	0.43
1:A:75:LEU:HA	1:A:75:LEU:HD23	1.79	0.43
1:B:234:ARG:HB2	1:B:314:ALA:O	2.18	0.43
1:E:262:LEU:HD23	1:E:262:LEU:N	2.33	0.43
1:F:50:PHE:C	1:F:50:PHE:CD1	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:SER:O	1:A:85:ARG:HG3	2.18	0.43
1:C:311:HIS:CD2	1:C:313:THR:HG23	2.53	0.43
1:C:20:THR:CG2	1:C:94:LEU:HB2	2.48	0.43
1:E:272:SER:HA	1:E:406:GLY:O	2.17	0.43
1:E:95:TRP:CD1	1:E:100:SER:HA	2.54	0.43
1:G:172:SER:HA	1:G:401:SER:OG	2.18	0.43
1:E:74:ARG:HA	1:E:77:MET:CG	2.48	0.43
1:F:222:GLU:OE1	1:F:225:ARG:HD3	2.19	0.43
1:H:375:THR:HA	1:H:376:PRO:HD2	1.88	0.43
1:A:112:VAL:HA	1:A:196:GLY:O	2.18	0.43
1:A:59:LYS:H	1:A:220:ASN:ND2	2.17	0.43
1:C:323:ALA:HA	1:C:382:LEU:HD11	2.00	0.43
1:E:130:ASN:HA	1:F:54:TRP:CH2	2.54	0.43
1:F:72:MET:CE	1:F:89:LEU:HB2	2.49	0.43
1:G:60:ILE:CG2	1:G:220:ASN:HA	2.48	0.43
1:G:222:GLU:OE1	1:G:225:ARG:HD3	2.18	0.43
1:D:295:LEU:CD2	1:D:305:ILE:HD11	2.49	0.43
1:E:63:HIS:HE1	1:E:202:ILE:HB	1.84	0.43
1:F:171:GLN:HG3	1:F:347:ILE:HG23	2.01	0.43
1:F:380:ILE:O	1:F:381:ASP:HB3	2.19	0.43
1:C:50:PHE:CD1	1:C:50:PHE:C	2.92	0.43
1:F:327:ARG:NH1	1:F:380:ILE:O	2.51	0.43
1:B:313:THR:HA	1:B:340:LYS:HD2	1.99	0.43
1:B:263:ALA:HB3	1:B:359:VAL:HG22	2.01	0.43
1:B:50:PHE:C	1:B:50:PHE:CD1	2.92	0.43
1:B:272:SER:HA	1:B:406:GLY:O	2.19	0.43
1:D:377:ASP:HB3	1:D:380:ILE:CG1	2.49	0.43
1:F:353:LEU:O	1:F:357:LEU:HG	2.19	0.43
1:A:141:ALA:O	1:A:145:ILE:HG13	2.19	0.42
1:B:27:PRO:HG3	1:B:66:ASP:CB	2.48	0.42
1:D:228:ARG:O	1:D:234:ARG:HB3	2.18	0.42
1:D:95:TRP:CD1	1:D:100:SER:HA	2.54	0.42
1:E:60:ILE:HG12	1:E:220:ASN:ND2	2.33	0.42
1:F:377:ASP:HA	1:F:378:PRO:HD2	1.83	0.42
1:G:104:ASP:HA	1:G:105:PRO:HD2	1.81	0.42
1:G:146:MET:HA	1:G:147:PRO:HD3	1.94	0.42
1:G:168:VAL:O	1:H:148:ASN:HB3	2.19	0.42
1:H:168:VAL:HG23	1:H:168:VAL:O	2.18	0.42
1:H:260:LYS:HA	1:H:261:PRO:HD3	1.85	0.42
1:G:26:SER:OG	1:G:31:SER:HB2	2.19	0.42
1:E:75:LEU:HA	1:E:75:LEU:HD23	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:377:ASP:OD1	1:F:379:GLU:HB2	2.19	0.42
1:A:307:HIS:HE1	1:A:337:TYR:HB3	1.84	0.42
1:B:260:LYS:HD2	1:B:261:PRO:HD2	2.01	0.42
1:C:279:ALA:HA	1:C:280:PRO:HD3	1.85	0.42
1:D:377:ASP:HA	1:D:378:PRO:HD2	1.90	0.42
1:G:279:ALA:HA	1:G:280:PRO:HD3	1.94	0.42
1:G:3:GLN:HA	1:G:4:PRO:HD2	1.86	0.42
1:D:26:SER:OG	1:D:27:PRO:HD2	2.20	0.42
1:E:347:ILE:HG22	1:E:348:GLY:N	2.34	0.42
1:B:340:LYS:HE3	1:B:350:VAL:HG21	2.01	0.42
1:E:146:MET:HA	1:E:147:PRO:HD3	1.78	0.42
1:C:356:VAL:O	1:C:360:LEU:HG	2.19	0.42
1:F:264:ARG:HG3	1:F:416:TYR:HA	2.01	0.42
1:H:402:PHE:HA	1:H:407:HIS:O	2.19	0.42
1:A:13:SER:O	1:A:250:THR:HA	2.20	0.42
1:C:122:ILE:HG12	1:C:145:ILE:HD13	2.00	0.42
1:E:216:MET:HE2	1:E:216:MET:HB3	1.91	0.42
1:H:313:THR:CG2	1:H:313:THR:O	2.67	0.42
1:B:232:LYS:HE3	1:B:378:PRO:HD2	2.02	0.42
1:B:56:LEU:O	1:B:59:LYS:HE3	2.19	0.42
1:D:219:ARG:HD2	1:D:226:ALA:HA	2.02	0.42
1:D:21:ALA:HB3	1:D:29:ILE:HD13	2.02	0.42
1:G:54:TRP:HB3	1:H:134:PRO:HG3	2.01	0.42
1:H:157:GLN:HE21	1:H:157:GLN:HB3	1.66	0.42
1:H:229:PRO:HD3	1:H:314:ALA:HB2	2.02	0.42
1:E:150:ALA:O	1:E:154:ILE:HG13	2.20	0.41
1:E:171:GLN:HG2	1:E:345:HIS:NE2	2.35	0.41
1:F:221:ASP:N	1:F:221:ASP:OD1	2.42	0.41
1:H:347:ILE:HG22	1:H:348:GLY:N	2.35	0.41
1:B:402:PHE:HD1	1:B:408:ASN:HA	1.85	0.41
1:C:350:VAL:O	1:C:354:GLU:HG3	2.20	0.41
1:F:176:GLU:HG2	1:F:180:HIS:HD2	1.85	0.41
1:H:313:THR:HG23	1:H:313:THR:O	2.20	0.41
1:B:110:VAL:HG23	1:B:160:ALA:CB	2.50	0.41
1:D:268:ALA:O	1:D:297:LEU:HD12	2.20	0.41
1:E:111:VAL:O	1:E:195:CYS:HA	2.21	0.41
1:E:283:ASP:OD1	1:E:284:GLY:N	2.53	0.41
1:E:168:VAL:HG21	1:F:147:PRO:HB2	2.03	0.41
1:F:46:LEU:HB3	1:F:51:VAL:HG21	2.02	0.41
1:G:265:LEU:HD11	1:G:411:LEU:HD22	2.02	0.41
1:C:60:ILE:HG23	1:C:220:ASN:HD22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:ALA:HA	1:D:280:PRO:HD3	1.77	0.41
1:G:314:ALA:HA	1:G:319:ASP:OD2	2.21	0.41
1:G:68:VAL:HG22	1:G:89:LEU:HD23	2.02	0.41
1:H:272:SER:HA	1:H:406:GLY:O	2.19	0.41
1:D:219:ARG:HH11	1:D:225:ARG:HH12	1.68	0.41
1:F:30:GLU:O	1:F:34:LYS:HG3	2.20	0.41
1:G:22:THR:O	1:G:242:ALA:HA	2.21	0.41
1:H:59:LYS:H	1:H:220:ASN:HD21	1.69	0.41
1:B:112:VAL:HA	1:B:196:GLY:O	2.20	0.41
1:B:33:TRP:O	1:B:37:LEU:HG	2.19	0.41
1:C:15:VAL:HB	1:C:261:PRO:HB3	2.03	0.41
1:E:231:ASP:O	1:E:234:ARG:HG2	2.21	0.41
1:G:176:GLU:HG2	1:G:180:HIS:HD2	1.85	0.41
1:A:60:ILE:HG12	1:A:220:ASN:HD22	1.86	0.41
1:B:199:GLU:HG2	1:B:346:SER:O	2.20	0.41
1:C:110:VAL:HG21	1:C:155:GLY:HA2	2.02	0.41
1:F:181:ALA:O	1:F:185:ILE:HG13	2.21	0.41
1:H:129:MET:HA	1:H:133:GLY:O	2.20	0.41
1:B:229:PRO:HA	1:B:319:ASP:OD2	2.21	0.41
1:C:119:ALA:O	1:C:122:ILE:HB	2.21	0.41
1:G:313:THR:HG22	1:G:345:HIS:CD2	2.55	0.41
1:G:407:HIS:NE2	1:H:148:ASN:ND2	2.60	0.41
1:H:293:ARG:O	1:H:293:ARG:HD2	2.20	0.41
1:B:170:ALA:HB1	1:B:171:GLN:OE1	2.21	0.41
1:D:8:ASN:OD1	1:D:8:ASN:C	2.59	0.41
1:E:75:LEU:CD2	1:E:79:ARG:HD2	2.51	0.41
1:F:115:GLY:HA3	1:F:199:GLU:OE1	2.21	0.41
1:F:54:TRP:O	1:F:55:ASP:C	2.59	0.41
1:C:138:SER:HA	1:C:139:PRO:HD3	1.89	0.40
1:C:314:ALA:HA	1:C:319:ASP:OD2	2.20	0.40
1:C:337:TYR:HB2	1:C:367:ILE:CG2	2.51	0.40
1:D:4:PRO:HB2	1:D:11:PHE:CZ	2.56	0.40
1:E:101:PRO:HG3	1:E:257:ARG:NH2	2.36	0.40
1:F:196:GLY:HA3	1:F:245:LEU:HD23	2.03	0.40
1:G:174:GLY:O	1:G:178:ILE:HG13	2.22	0.40
1:G:229:PRO:HD2	1:G:341:SER:HB3	2.03	0.40
1:A:301:SER:O	1:A:304:ASP:HB2	2.21	0.40
1:B:307:HIS:O	1:B:397:ALA:HA	2.21	0.40
1:E:25:ILE:HD12	1:E:343:LEU:HD21	2.02	0.40
1:F:146:MET:HA	1:F:147:PRO:HD3	1.92	0.40
1:F:338:ALA:HB3	1:F:370:THR:CG2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:VAL:O	1:B:146:MET:HE3	2.22	0.40
1:C:176:GLU:HB2	1:C:409:VAL:HG21	2.03	0.40
1:C:338:ALA:HA	1:C:339:PRO:HD2	1.85	0.40
1:E:225:ARG:HA	1:E:372:ASN:OD1	2.21	0.40
1:G:388:GLU:HG3	1:G:389:PRO:HD2	2.02	0.40
1:B:146:MET:HE3	1:B:146:MET:HB3	1.88	0.40
1:B:66:ASP:OD2	1:B:71:HIS:HE1	2.03	0.40
1:E:75:LEU:HD21	1:E:79:ARG:HD2	2.03	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	413/416 (99%)	395 (96%)	17 (4%)	1 (0%)	47	46
1	B	414/416 (100%)	398 (96%)	14 (3%)	2 (0%)	29	22
1	C	413/416 (99%)	398 (96%)	13 (3%)	2 (0%)	29	22
1	D	414/416 (100%)	398 (96%)	14 (3%)	2 (0%)	29	22
1	E	413/416 (99%)	391 (95%)	19 (5%)	3 (1%)	22	15
1	F	413/416 (99%)	386 (94%)	22 (5%)	5 (1%)	13	7
1	G	413/416 (99%)	389 (94%)	20 (5%)	4 (1%)	15	9
1	H	414/416 (100%)	394 (95%)	18 (4%)	2 (0%)	29	22
All	All	3307/3328 (99%)	3149 (95%)	137 (4%)	21 (1%)	25	18

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	312	GLY
1	F	314	ALA

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Mol	Chain	Res	Type
1	C	312	GLY
1	D	312	GLY
1	D	347	ILE
1	E	312	GLY
1	E	383	ASP
1	F	347	ILE
1	G	312	GLY
1	H	312	GLY
1	E	347	ILE
1	F	381	ASP
1	G	347	ILE
1	A	347	ILE
1	B	347	ILE
1	C	347	ILE
1	F	55	ASP
1	H	347	ILE
1	G	170	ALA
1	G	314	ALA
1	B	312	GLY

### 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	307/308 (100%)	296 (96%)	11 (4%)	35	33
1	B	308/308 (100%)	299 (97%)	9 (3%)	42	42
1	C	307/308 (100%)	300 (98%)	7 (2%)	50	53
1	D	308/308 (100%)	298 (97%)	10 (3%)	39	38
1	E	307/308 (100%)	295 (96%)	12 (4%)	32	30
1	F	307/308 (100%)	293 (95%)	14 (5%)	27	23
1	G	307/308 (100%)	296 (96%)	11 (4%)	35	33
1	H	308/308 (100%)	299 (97%)	9 (3%)	42	42
All	All	2459/2464 (100%)	2376 (97%)	83 (3%)	37	35

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	48	ASP
1	A	74	ARG
1	A	116	LEU
1	A	120	GLU
1	A	129	MET
1	A	205	LEU
1	A	239	PHE
1	A	255	LYS
1	A	388	GLU
1	A	401	SER
1	B	3	GLN
1	B	48	ASP
1	B	75	LEU
1	B	96	GLU
1	B	114	THR
1	B	116	LEU
1	B	128	LEU
1	B	136	LYS
1	B	375	THR
1	C	49	GLU
1	C	116	LEU
1	C	120	GLU
1	C	239	PHE
1	C	388	GLU
1	C	395	ARG
1	C	401	SER
1	D	3	GLN
1	D	28	ASP
1	D	52	THR
1	D	74	ARG
1	D	75	LEU
1	D	96	GLU
1	D	116	LEU
1	D	128	LEU
1	D	136	LYS
1	D	192	VAL
1	E	49	GLU
1	E	75	LEU
1	E	114	THR
1	E	116	LEU
1	E	120	GLU

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Mol	Chain	Res	Type
1	E	142	VAL
1	E	214	ARG
1	E	227	SER
1	E	252	GLU
1	E	255	LYS
1	E	379	GLU
1	E	395	ARG
1	F	3	GLN
1	F	53	LYS
1	F	60	ILE
1	F	68	VAL
1	F	75	LEU
1	F	78	ARG
1	F	128	LEU
1	F	136	LYS
1	F	153	VAL
1	F	221	ASP
1	F	239	PHE
1	F	350	VAL
1	F	360	LEU
1	F	379	GLU
1	G	114	THR
1	G	116	LEU
1	G	120	GLU
1	G	146	MET
1	G	205	LEU
1	G	211	SER
1	G	219	ARG
1	G	224	GLU
1	G	239	PHE
1	G	255	LYS
1	G	350	VAL
1	H	3	GLN
1	H	49	GLU
1	H	75	LEU
1	H	128	LEU
1	H	136	LYS
1	H	218	THR
1	H	239	PHE
1	H	255	LYS
1	H	313	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	220	ASN
1	A	399	ASN
1	B	71	HIS
1	B	157	GLN
1	B	220	ASN
1	C	220	ASN
1	D	157	GLN
1	D	399	ASN
1	D	408	ASN
1	E	220	ASN
1	F	71	HIS
1	F	157	GLN
1	F	180	HIS
1	F	220	ASN
1	F	399	ASN
1	G	71	HIS
1	G	157	GLN
1	G	180	HIS
1	G	399	ASN
1	H	71	HIS
1	H	157	GLN
1	H	180	HIS
1	H	220	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PG4	A	1418	-	12,12,12	0.51	0	11,11,11	0.57	0
3	PG4	F	1417	-	12,12,12	0.53	0	11,11,11	0.32	0
4	PEG	D	1418	-	6,6,6	0.55	0	5,5,5	0.15	0
3	PG4	C	1417	-	12,12,12	0.53	0	11,11,11	0.37	0
3	PG4	B	1418	-	12,12,12	0.52	0	11,11,11	0.47	0
3	PG4	E	1417	-	12,12,12	0.51	0	11,11,11	0.37	0
3	PG4	D	1417	-	12,12,12	0.50	0	11,11,11	0.43	0
3	PG4	B	1417	-	12,12,12	0.47	0	11,11,11	0.48	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	PG4	A	1418	-	-	5/10/10/10	-
3	PG4	F	1417	-	-	7/10/10/10	-
4	PEG	D	1418	-	-	1/4/4/4	-
3	PG4	C	1417	-	-	5/10/10/10	-
3	PG4	B	1418	-	-	5/10/10/10	-
3	PG4	E	1417	-	-	3/10/10/10	-
3	PG4	D	1417	-	-	4/10/10/10	-
3	PG4	B	1417	-	-	4/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1417	PG4	O3-C5-C6-O4
3	B	1418	PG4	O2-C3-C4-O3
3	C	1417	PG4	O4-C7-C8-O5
3	A	1418	PG4	O2-C3-C4-O3
3	F	1417	PG4	O3-C5-C6-O4
3	B	1418	PG4	O3-C5-C6-O4
3	A	1418	PG4	O1-C1-C2-O2
3	B	1417	PG4	O1-C1-C2-O2
4	D	1418	PEG	O2-C3-C4-O4
3	B	1418	PG4	O1-C1-C2-O2
3	A	1418	PG4	C5-C6-O4-C7
3	D	1417	PG4	C6-C5-O3-C4
3	F	1417	PG4	C8-C7-O4-C6
3	E	1417	PG4	C3-C4-O3-C5
3	F	1417	PG4	C6-C5-O3-C4
3	C	1417	PG4	C4-C3-O2-C2
3	B	1418	PG4	C4-C3-O2-C2
3	D	1417	PG4	C4-C3-O2-C2
3	E	1417	PG4	C8-C7-O4-C6
3	B	1418	PG4	C5-C6-O4-C7
3	D	1417	PG4	O4-C7-C8-O5
3	A	1418	PG4	C3-C4-O3-C5
3	F	1417	PG4	O2-C3-C4-O3
3	D	1417	PG4	C3-C4-O3-C5
3	C	1417	PG4	C8-C7-O4-C6
3	F	1417	PG4	C5-C6-O4-C7
3	B	1417	PG4	C1-C2-O2-C3
3	B	1417	PG4	O2-C3-C4-O3
3	A	1418	PG4	O3-C5-C6-O4
3	C	1417	PG4	C6-C5-O3-C4
3	F	1417	PG4	O4-C7-C8-O5
3	F	1417	PG4	O1-C1-C2-O2
3	E	1417	PG4	O2-C3-C4-O3
3	C	1417	PG4	O2-C3-C4-O3

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1418	PG4	2	0
3	F	1417	PG4	1	0
3	C	1417	PG4	1	0
3	E	1417	PG4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1417	PG4	1	0
3	B	1417	PG4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	415/416 (99%)	-0.70	2 (0%) 91 93	44, 52, 64, 80	0
1	B	415/416 (99%)	-0.72	0 100 100	43, 52, 63, 82	0
1	C	415/416 (99%)	-0.72	1 (0%) 95 96	43, 49, 60, 85	0
1	D	415/416 (99%)	-0.75	0 100 100	40, 48, 58, 79	0
1	E	415/416 (99%)	-0.65	1 (0%) 95 96	48, 54, 65, 86	0
1	F	415/416 (99%)	-0.46	1 (0%) 95 96	48, 60, 71, 88	0
1	G	415/416 (99%)	-0.55	1 (0%) 95 96	49, 59, 71, 93	0
1	H	415/416 (99%)	-0.69	0 100 100	46, 54, 65, 81	0
All	All	3320/3328 (99%)	-0.65	6 (0%) 95 96	40, 54, 67, 93	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	SER	4.6
1	E	2	SER	4.0
1	G	3	GLN	3.5
1	A	2	SER	2.6
1	F	2	SER	2.5
1	A	74	ARG	2.4

### 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

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( $\text{\AA}^2$ )	Q<0.9
3	PG4	A	1418	13/13	0.92	0.12	51,57,63,64	0
3	PG4	B	1417	13/13	0.92	0.18	51,59,62,66	0
3	PG4	C	1417	13/13	0.94	0.09	47,57,66,69	0
4	PEG	D	1418	7/7	0.94	0.10	49,50,51,55	0
3	PG4	B	1418	13/13	0.95	0.10	53,58,63,67	0
3	PG4	E	1417	13/13	0.95	0.09	53,60,63,64	0
3	PG4	F	1417	13/13	0.95	0.10	55,59,62,64	0
3	PG4	D	1417	13/13	0.97	0.11	47,52,56,58	0
2	NA	G	1417	1/1	0.98	0.18	56,56,56,56	0
2	NA	H	1417	1/1	0.99	0.18	49,49,49,49	0
2	NA	D	1419	1/1	0.99	0.16	42,42,42,42	0
2	NA	B	1419	1/1	0.99	0.21	48,48,48,48	0
2	NA	A	1417	1/1	0.99	0.18	49,49,49,49	0
2	NA	E	1418	1/1	0.99	0.14	43,43,43,43	0
2	NA	F	1418	1/1	0.99	0.12	52,52,52,52	0
2	NA	C	1418	1/1	1.00	0.17	44,44,44,44	0

## 6.5 Other polymers

There are no such residues in this entry.