



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:08 PM GMT

PDB ID : 3SY9  
Title : Crystal structure of Pseudomonas aeruginosa OccD2 (OpdC)  
Authors : van den Berg, B.; Eren, E.  
Deposited on : 2011-07-16  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

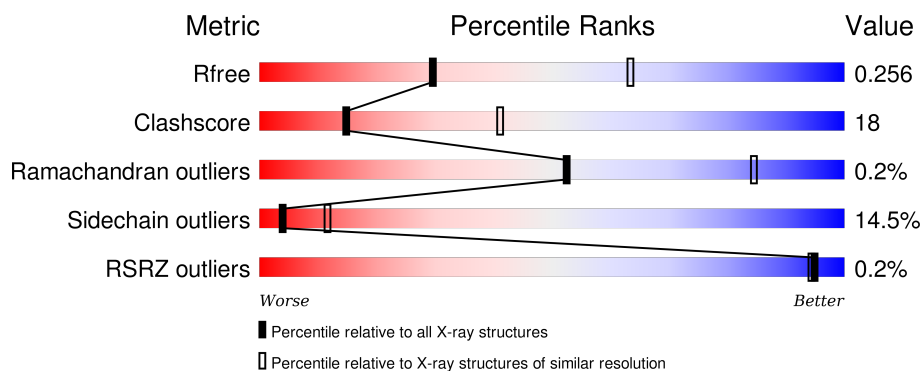
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	430	<div> <div>50%</div> <div>31%</div> <div>5%</div> <div>14%</div> </div>
1	B	430	<div> <div>56%</div> <div>25%</div> <div>5%</div> <div>13%</div> </div>
1	C	430	<div> <div>56%</div> <div>23%</div> <div>•</div> <div>16%</div> </div>
1	D	430	<div> <div>57%</div> <div>20%</div> <div>6%</div> <div>16%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	C8E	A	501	-	-	-	X
2	C8E	A	502	-	-	-	X
2	C8E	A	503	-	-	-	X
2	C8E	A	504	-	-	-	X
2	C8E	A	505	-	-	-	X
2	C8E	B	502	-	-	-	X
2	C8E	B	503	-	-	-	X
2	C8E	B	504	-	-	-	X
2	C8E	B	505	-	-	-	X
2	C8E	B	506	-	-	-	X
2	C8E	C	502	-	-	-	X
2	C8E	C	503	-	-	-	X
3	BOG	A	506	X	-	-	-
3	BOG	B	507	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11713 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 Histidine porin OpdC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2874	1830	477	565	2			
1	B	372	Total	C	N	O	S	0	0	0
			2886	1838	480	566	2			
1	C	360	Total	C	N	O	S	0	0	0
			2767	1761	459	545	2			
1	D	361	Total	C	N	O	S	0	0	0
			2770	1760	458	550	2			

There are 36 discrepancies between the modelled and reference sequences:

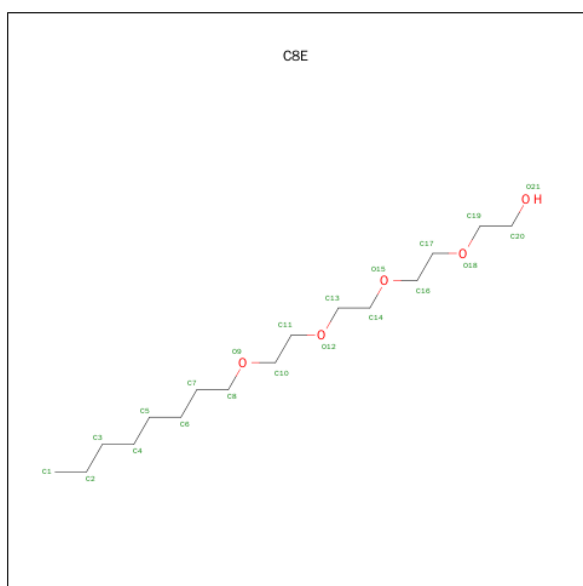
Chain	Residue	Modelled	Actual	Comment	Reference
A	328	VAL	LEU	SEE REMARK 999	UNP Q9I6X0
A	423	GLY	-	EXPRESSION TAG	UNP Q9I6X0
A	424	GLY	-	EXPRESSION TAG	UNP Q9I6X0
A	425	HIS	-	EXPRESSION TAG	UNP Q9I6X0
A	426	HIS	-	EXPRESSION TAG	UNP Q9I6X0
A	427	HIS	-	EXPRESSION TAG	UNP Q9I6X0
A	428	HIS	-	EXPRESSION TAG	UNP Q9I6X0
A	429	HIS	-	EXPRESSION TAG	UNP Q9I6X0
A	430	HIS	-	EXPRESSION TAG	UNP Q9I6X0
B	328	VAL	LEU	SEE REMARK 999	UNP Q9I6X0
B	423	GLY	-	EXPRESSION TAG	UNP Q9I6X0
B	424	GLY	-	EXPRESSION TAG	UNP Q9I6X0
B	425	HIS	-	EXPRESSION TAG	UNP Q9I6X0
B	426	HIS	-	EXPRESSION TAG	UNP Q9I6X0
B	427	HIS	-	EXPRESSION TAG	UNP Q9I6X0
B	428	HIS	-	EXPRESSION TAG	UNP Q9I6X0
B	429	HIS	-	EXPRESSION TAG	UNP Q9I6X0
B	430	HIS	-	EXPRESSION TAG	UNP Q9I6X0
C	328	VAL	LEU	SEE REMARK 999	UNP Q9I6X0
C	423	GLY	-	EXPRESSION TAG	UNP Q9I6X0
C	424	GLY	-	EXPRESSION TAG	UNP Q9I6X0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	425	HIS	-	EXPRESSION TAG	UNP Q9I6X0
C	426	HIS	-	EXPRESSION TAG	UNP Q9I6X0
C	427	HIS	-	EXPRESSION TAG	UNP Q9I6X0
C	428	HIS	-	EXPRESSION TAG	UNP Q9I6X0
C	429	HIS	-	EXPRESSION TAG	UNP Q9I6X0
C	430	HIS	-	EXPRESSION TAG	UNP Q9I6X0
D	328	VAL	LEU	SEE REMARK 999	UNP Q9I6X0
D	423	GLY	-	EXPRESSION TAG	UNP Q9I6X0
D	424	GLY	-	EXPRESSION TAG	UNP Q9I6X0
D	425	HIS	-	EXPRESSION TAG	UNP Q9I6X0
D	426	HIS	-	EXPRESSION TAG	UNP Q9I6X0
D	427	HIS	-	EXPRESSION TAG	UNP Q9I6X0
D	428	HIS	-	EXPRESSION TAG	UNP Q9I6X0
D	429	HIS	-	EXPRESSION TAG	UNP Q9I6X0
D	430	HIS	-	EXPRESSION TAG	UNP Q9I6X0

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



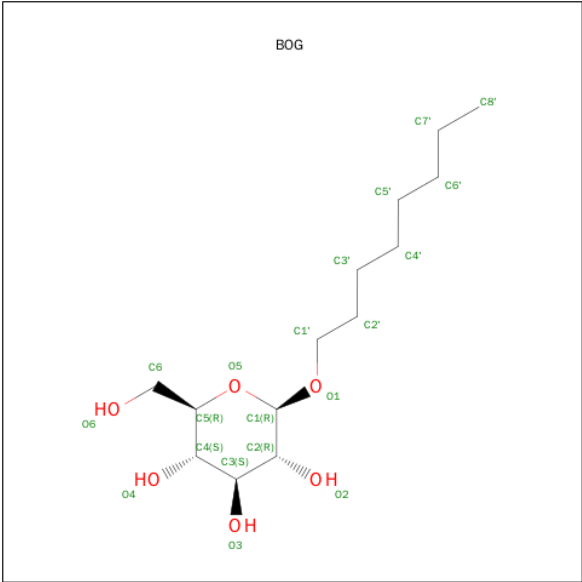
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	9	5		
2	A	1	Total	C	O	0	0
			12	10	2		
2	A	1	Total	C	O	0	0
			16	11	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	13	3		
2	A	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			10	9	1		
2	B	1	Total	C	O	0	0
			16	11	5		
2	B	1	Total	C	O	0	0
			15	12	3		
2	B	1	Total	C	O	0	0
			16	13	3		
2	B	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			11	10	1		
2	C	1	Total	C	O	0	0
			9	6	3		
2	C	1	Total	C	O	0	0
			16	13	3		
2	C	1	Total	C	O	0	0
			18	13	5		
2	C	1	Total	C	O	0	0
			11	10	1		
2	C	1	Total	C		0	0
			8	8			
2	D	1	Total	C	O	0	0
			10	9	1		
2	D	1	Total	C	O	0	0
			12	8	4		

- Molecule 3 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			15	9	6		

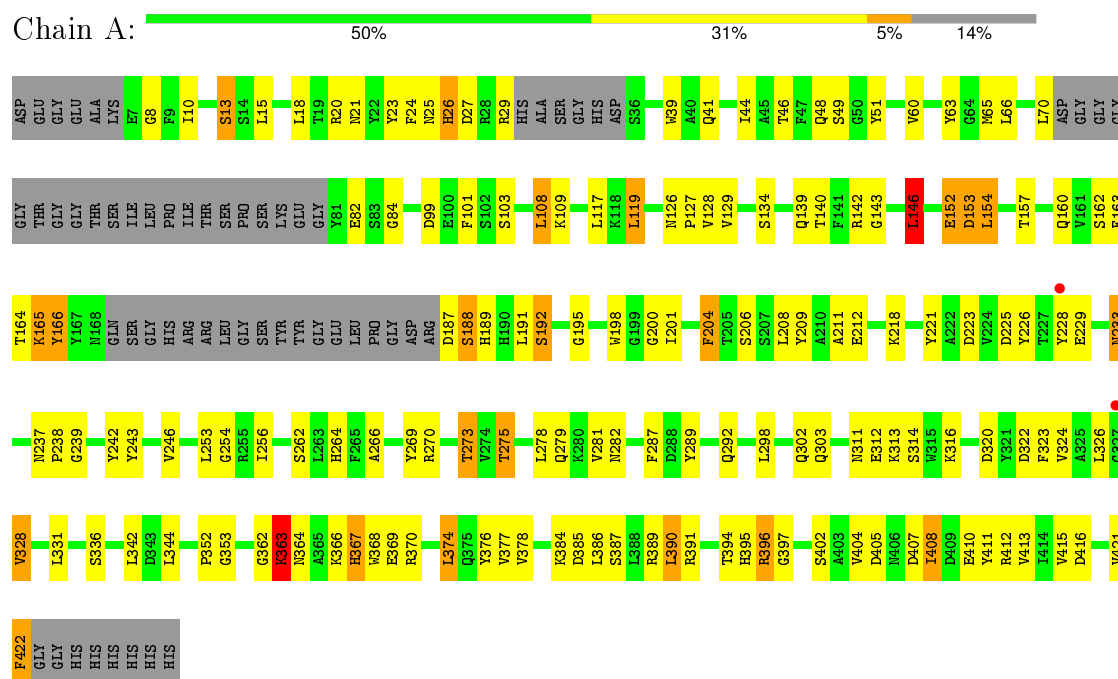
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	32	Total	O	0	0
			32	32		
4	C	32	Total	O	0	0
			32	32		
4	D	27	Total	O	0	0
			27	27		

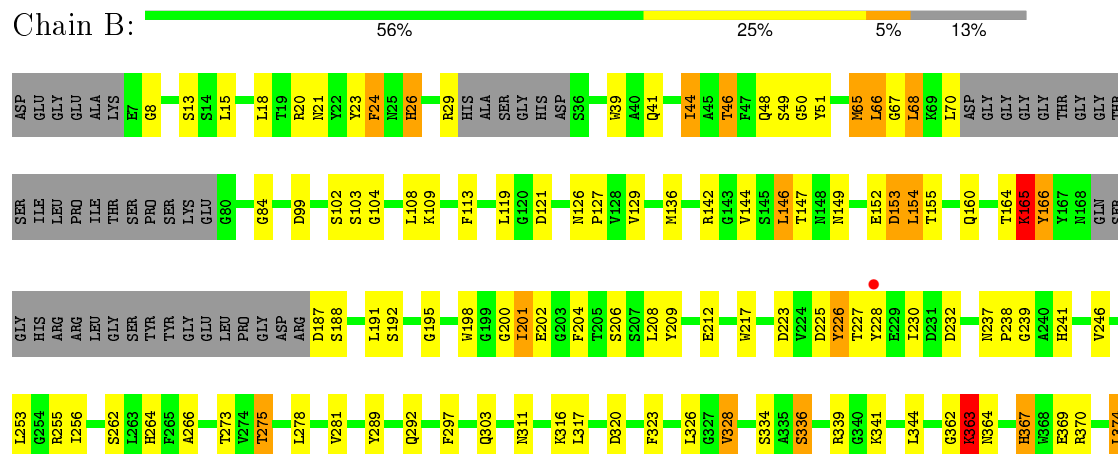
### 3 Residue-property plots

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



#### • Molecule 1: Histidine porin OpdC







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.35Å 102.83Å 101.70Å 77.67° 62.57° 62.95°	Depositor
Resolution (Å)	14.96 – 2.80 40.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (14.96-2.80) 89.6 (40.92-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.216 , 0.266 0.210 , 0.256	Depositor DCC
$R_{free}$ test set	1988 reflections (3.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.5	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.7	EDS
Estimated twinning fraction	0.000 for h,h-l,k 0.000 for h,l,h-k 0.458 for h,h-k,h-l 0.000 for -h,-k,-h+l 0.000 for -h,-h+k,-l 0.002 for -h,-l,-k 0.002 for -h,-h+l,-h+k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 71926 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11713	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: C8E, BOG

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	0.43	0/2950	0.63	1/4011 (0.0%)
1	B	0.44	0/2962	0.63	0/4026
1	C	0.41	0/2839	0.63	1/3863 (0.0%)
1	D	0.42	0/2843	0.64	0/3871
All	All	0.42	0/11594	0.63	2/15771 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	LEU	CA-CB-CG	5.49	127.94	115.30
1	A	146	LEU	CA-CB-CG	5.45	127.83	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	LYS	Peptide
1	A	84	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	165	LYS	Peptide
1	B	166	TYR	Peptide
1	B	84	GLY	Peptide

## 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	2874	0	2624	120	0
1	B	2886	0	2642	115	0
1	C	2767	0	2496	78	0
1	D	2770	0	2497	78	0
2	A	79	0	118	2	0
2	B	89	0	141	5	0
2	C	62	0	95	2	0
2	D	22	0	32	1	0
3	A	16	0	17	2	0
3	B	15	0	15	6	0
4	A	42	0	0	6	0
4	B	32	0	0	1	0
4	C	32	0	0	3	0
4	D	27	0	0	0	0
All	All	11713	0	10677	393	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 18.

All (393) 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:201:ILE:HG21	1:B:204:PHE:HB3	1.17	1.10
1:A:103:SER:HA	3:A:506:BOG:H1	1.32	1.04
1:C:201:ILE:HG22	1:C:202:GLU:H	1.25	0.99
1:A:41:GLN:HG2	1:A:70:LEU:HD11	1.51	0.92
1:D:148:ASN:HD21	1:D:150:SER:HB2	1.37	0.89
1:B:24:PHE:HB2	1:B:412:ARG:HG2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ILE:HG22	1:D:202:GLU:H	1.36	0.88
1:C:18:LEU:HB3	1:C:44:ILE:HG23	1.55	0.86
1:C:201:ILE:HG22	1:C:202:GLU:N	1.90	0.86
1:B:201:ILE:HG23	1:B:202:GLU:N	1.88	0.85
1:A:18:LEU:HB3	1:A:44:ILE:HG23	1.58	0.85
1:B:266:ALA:HB2	1:B:275:THR:HG23	1.55	0.85
1:B:103:SER:HA	3:B:507:BOG:O2	1.78	0.83
1:A:394:THR:HG23	1:A:396:ARG:HH11	1.43	0.83
1:A:266:ALA:HB2	1:A:275:THR:HG23	1.58	0.83
1:C:378:VAL:HG11	1:C:383:ALA:HB3	1.60	0.83
1:D:41:GLN:HG2	1:D:70:LEU:HD11	1.62	0.81
1:B:18:LEU:HB3	1:B:44:ILE:HG23	1.60	0.81
1:C:266:ALA:HB2	1:C:275:THR:HG23	1.61	0.81
1:B:201:ILE:CG2	1:B:204:PHE:HB3	2.07	0.80
1:D:266:ALA:HB2	1:D:275:THR:HG23	1.63	0.80
1:A:273:THR:HG23	1:A:320:ASP:HB2	1.63	0.78
1:A:289:TYR:CE1	1:A:292:GLN:HG2	2.19	0.78
1:D:23:TYR:HB3	1:D:413:VAL:HG12	1.66	0.78
1:A:370:ARG:O	4:A:639:HOH:O	2.02	0.78
1:D:18:LEU:HB3	1:D:44:ILE:HG23	1.65	0.77
1:B:20:ARG:HD3	1:B:416:ASP:OD2	1.84	0.76
1:B:289:TYR:CE1	1:B:292:GLN:HG2	2.21	0.76
1:B:104:GLY:N	3:B:507:BOG:O2	2.19	0.75
1:B:29:ARG:HH11	1:B:396:ARG:HH22	1.31	0.75
1:A:20:ARG:HD3	1:A:416:ASP:OD2	1.86	0.75
1:D:148:ASN:ND2	1:D:150:SER:H	1.84	0.75
1:C:139:GLN:HE21	1:C:291:ASN:HD21	1.35	0.74
1:A:103:SER:CA	3:A:506:BOG:H1	2.15	0.74
1:B:23:TYR:HD1	1:B:413:VAL:HG13	1.51	0.73
1:B:23:TYR:HB2	1:B:39:TRP:CE3	2.23	0.73
1:D:151:PHE:HB2	1:D:154:LEU:HD11	1.70	0.72
1:C:20:ARG:HD3	1:C:416:ASP:OD2	1.89	0.72
1:B:323:PHE:HB3	1:B:328:VAL:HG23	1.72	0.72
1:B:41:GLN:HG2	1:B:70:LEU:HD11	1.71	0.72
1:B:164:THR:C	1:B:165:LYS:HG2	2.10	0.71
1:A:164:THR:OG1	1:A:165:LYS:N	2.24	0.71
1:A:384:LYS:O	1:A:385:ASP:HB2	1.90	0.70
1:C:39:TRP:CD1	1:C:70:LEU:HD12	2.27	0.69
1:D:20:ARG:HD3	1:D:416:ASP:OD2	1.93	0.69
1:A:8:GLY:HA2	1:A:51:TYR:O	1.94	0.68
1:D:17:LEU:HD11	1:D:43:PHE:CD2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:PHE:HB3	1:A:328:VAL:HG23	1.76	0.68
1:D:409:ASP:OD2	1:D:409:ASP:N	2.26	0.67
1:B:21:ASN:HB2	1:B:415:VAL:HB	1.77	0.67
1:C:303:GLN:OE1	4:C:632:HOH:O	2.10	0.67
1:A:394:THR:HB	4:A:639:HOH:O	1.95	0.67
1:B:67:GLY:C	1:B:68:LEU:HD12	2.15	0.67
1:C:162:SER:HA	1:C:189:HIS:O	1.95	0.67
1:B:201:ILE:HG21	1:B:204:PHE:CB	2.11	0.66
1:B:389:ARG:HE	1:B:391:ARG:HD2	1.60	0.65
1:B:8:GLY:O	1:B:50:GLY:HA3	1.96	0.65
1:B:344:LEU:HB2	1:B:362:GLY:HA3	1.78	0.64
1:B:395:HIS:HB3	1:B:408:ILE:HD13	1.81	0.63
1:A:139:GLN:NE2	1:A:163:PHE:CD2	2.66	0.63
1:B:201:ILE:CG2	1:B:202:GLU:N	2.59	0.63
1:B:198:TRP:CZ2	1:B:200:GLY:HA3	2.34	0.63
1:C:41:GLN:CG	1:C:70:LEU:HD11	2.27	0.63
1:D:391:ARG:HB2	1:D:412:ARG:HB2	1.81	0.63
1:B:367:HIS:HA	1:B:397:GLY:HA2	1.81	0.62
1:D:201:ILE:HG22	1:D:202:GLU:N	2.13	0.62
1:B:395:HIS:HB3	1:B:408:ILE:CD1	2.28	0.62
1:C:191:LEU:HD23	1:C:191:LEU:C	2.20	0.62
1:A:187:ASP:CG	1:A:188:SER:H	2.03	0.62
1:B:266:ALA:CB	1:B:275:THR:HG23	2.29	0.62
1:A:82:GLU:HA	1:A:166:TYR:O	2.00	0.62
1:B:103:SER:HA	3:B:507:BOG:H1	1.81	0.61
1:C:66:LEU:HD12	1:C:102:SER:HB3	1.81	0.61
1:C:322:ASP:OD1	1:C:324:VAL:HG23	2.01	0.61
1:D:312:GLU:OE2	1:D:367:HIS:NE2	2.21	0.61
1:A:21:ASN:HB2	1:A:415:VAL:HB	1.81	0.61
1:D:323:PHE:HB3	1:D:328:VAL:HG23	1.81	0.61
1:C:377:VAL:HG22	1:C:387:SER:HB2	1.83	0.61
1:C:23:TYR:HB3	1:C:413:VAL:HG13	1.81	0.61
1:A:152:GLU:O	1:A:153:ASP:OD2	2.18	0.61
1:D:380:GLY:HA2	1:D:384:LYS:HG3	1.83	0.60
1:B:394:THR:HG23	1:B:396:ARG:HH11	1.65	0.60
1:C:148:ASN:HD21	1:C:150:SER:HB2	1.66	0.60
1:B:121:ASP:OD2	1:B:142:ARG:HG3	2.01	0.60
1:A:119:LEU:N	1:A:119:LEU:HD12	2.17	0.60
1:A:226:TYR:O	1:A:238:PRO:HD2	2.01	0.60
1:C:15:LEU:HD23	1:C:421:VAL:CG2	2.31	0.60
1:B:226:TYR:HD1	1:B:227:THR:N	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ASN:ND2	1:D:150:SER:HB2	2.13	0.60
1:B:326:LEU:O	1:B:326:LEU:HD23	2.02	0.60
1:D:151:PHE:HB2	1:D:154:LEU:CD1	2.31	0.60
1:C:391:ARG:HB2	1:C:412:ARG:HB2	1.82	0.60
1:B:160:GLN:HG2	1:B:192:SER:HB3	1.84	0.60
1:D:162:SER:HA	1:D:189:HIS:O	2.01	0.60
1:A:233:ASN:HB3	1:A:270:ARG:HG3	1.83	0.60
1:B:103:SER:CA	3:B:507:BOG:O2	2.48	0.60
1:A:239:GLY:HA3	1:A:264:HIS:CE1	2.36	0.60
1:C:45:ALA:O	1:C:63:TYR:HA	2.02	0.60
1:B:68:LEU:HD12	1:B:68:LEU:N	2.17	0.60
1:C:15:LEU:HD23	1:C:421:VAL:HG22	1.82	0.60
1:B:20:ARG:NH1	1:B:416:ASP:OD1	2.36	0.59
1:C:148:ASN:ND2	1:C:150:SER:H	2.00	0.59
1:C:201:ILE:CG2	1:C:202:GLU:N	2.64	0.58
1:D:365:ALA:HA	1:D:399:GLY:O	2.02	0.58
1:C:139:GLN:NE2	1:C:291:ASN:HD21	1.99	0.58
1:A:24:PHE:CZ	1:A:26:HIS:CE1	2.91	0.58
1:B:164:THR:OG1	1:B:165:LYS:N	2.37	0.58
1:C:240:ALA:HB2	1:C:263:LEU:HD23	1.86	0.58
1:B:281:VAL:O	1:B:311:ASN:HA	2.03	0.58
1:C:44:ILE:HD13	1:C:65:MET:HG3	1.84	0.58
1:A:23:TYR:HB2	1:A:39:TRP:CZ3	2.39	0.57
1:C:18:LEU:HB3	1:C:44:ILE:CG2	2.29	0.57
1:A:326:LEU:HD23	1:A:326:LEU:O	2.05	0.57
1:B:374:LEU:HD12	1:B:374:LEU:H	1.68	0.57
1:B:29:ARG:NH1	1:B:396:ARG:HH22	2.02	0.57
1:A:367:HIS:HA	1:A:397:GLY:HA2	1.87	0.57
1:A:139:GLN:HE22	1:A:163:PHE:HD2	1.53	0.57
1:A:344:LEU:HB2	1:A:362:GLY:HA3	1.87	0.57
1:D:421:VAL:O	1:D:422:PHE:C	2.43	0.57
1:B:384:LYS:O	1:B:385:ASP:HB2	2.05	0.57
1:D:191:LEU:HD23	1:D:191:LEU:C	2.25	0.57
1:A:218:LYS:HE3	4:A:623:HOH:O	2.04	0.56
1:C:39:TRP:NE1	1:C:70:LEU:HD12	2.20	0.56
1:A:164:THR:O	1:A:165:LYS:HG3	2.06	0.56
1:A:395:HIS:C	1:A:396:ARG:HD2	2.26	0.55
1:D:39:TRP:CD1	1:D:70:LEU:HB2	2.42	0.55
1:B:362:GLY:O	1:B:363:LYS:CB	2.53	0.55
1:B:374:LEU:CD1	1:B:390:LEU:HB2	2.36	0.55
1:A:152:GLU:HG3	1:A:152:GLU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:ASN:ND2	1:D:39:TRP:CH2	2.75	0.55
1:A:374:LEU:CD1	1:A:390:LEU:HB2	2.37	0.55
1:C:207:SER:O	1:C:222:ALA:HA	2.07	0.55
1:B:20:ARG:HG2	1:B:136:MET:HG3	1.88	0.54
1:C:111:ARG:HB3	4:C:609:HOH:O	2.08	0.54
1:D:154:LEU:H	1:D:154:LEU:HD12	1.71	0.54
1:A:26:HIS:HE1	1:A:410:GLU:OE2	1.90	0.54
1:C:160:GLN:HG2	1:C:192:SER:OG	2.08	0.54
1:A:311:ASN:HB2	4:A:609:HOH:O	2.08	0.54
1:B:237:ASN:HB3	1:B:266:ALA:HB3	1.88	0.54
1:B:29:ARG:HH11	1:B:396:ARG:NH2	2.02	0.54
1:A:395:HIS:HB3	1:A:408:ILE:CD1	2.38	0.53
1:D:326:LEU:O	1:D:326:LEU:HD23	2.09	0.53
1:B:164:THR:O	1:B:165:LYS:HG2	2.07	0.53
1:C:231:ASP:HB2	1:C:233:ASN:H	1.73	0.53
1:D:148:ASN:ND2	1:D:150:SER:N	2.55	0.53
1:D:119:LEU:HD12	1:D:119:LEU:N	2.24	0.53
1:A:233:ASN:O	1:A:269:TYR:HA	2.08	0.53
1:A:316:LYS:HD2	1:A:336:SER:HB2	1.90	0.53
1:D:373:ASP:OD2	1:D:389:ARG:NH1	2.42	0.53
1:B:23:TYR:HB2	1:B:39:TRP:CZ3	2.44	0.53
1:A:25:ASN:HB3	1:A:411:TYR:HB3	1.91	0.53
1:C:128:VAL:HG21	1:C:211:ALA:HB2	1.91	0.53
1:A:164:THR:O	1:A:165:LYS:CG	2.57	0.53
1:B:241:HIS:HB2	1:B:262:SER:HB3	1.90	0.52
1:A:266:ALA:CB	1:A:275:THR:HG23	2.33	0.52
1:D:377:VAL:HG22	1:D:387:SER:HB2	1.91	0.52
1:D:166:TYR:CG	1:D:167:TYR:N	2.77	0.52
1:A:23:TYR:HD2	1:A:413:VAL:HG13	1.74	0.52
1:B:226:TYR:O	1:B:238:PRO:HD2	2.09	0.52
1:A:402:SER:HA	1:A:405:ASP:O	2.10	0.52
1:B:316:LYS:HD2	1:B:336:SER:HB2	1.92	0.52
1:A:394:THR:CG2	1:A:396:ARG:HH11	2.20	0.52
1:C:410:GLU:OE1	1:C:412:ARG:NE	2.43	0.52
1:D:344:LEU:HB2	1:D:362:GLY:HA3	1.92	0.52
1:B:24:PHE:CB	1:B:412:ARG:HG2	2.36	0.51
1:A:395:HIS:HB3	1:A:408:ILE:HD13	1.92	0.51
1:B:394:THR:HG23	1:B:396:ARG:NH1	2.26	0.51
1:A:152:GLU:O	1:A:153:ASP:CB	2.57	0.51
1:C:343:ASP:OD1	1:C:345:THR:OG1	2.19	0.51
1:C:326:LEU:O	1:C:326:LEU:HD23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:O	1:A:421:VAL:O	2.28	0.51
1:B:201:ILE:HG22	1:B:204:PHE:H	1.75	0.51
1:B:362:GLY:O	1:B:363:LYS:HB2	2.11	0.51
1:B:374:LEU:N	1:B:374:LEU:HD12	2.26	0.51
1:A:201:ILE:HD12	1:A:204:PHE:CD2	2.46	0.51
1:A:160:GLN:HG2	1:A:192:SER:HB3	1.93	0.51
1:A:394:THR:HG23	1:A:396:ARG:NH1	2.19	0.51
1:B:160:GLN:HG2	1:B:192:SER:CB	2.40	0.51
1:D:148:ASN:HD21	1:D:150:SER:H	1.56	0.51
1:A:369:GLU:HA	1:A:394:THR:O	2.10	0.51
1:D:374:LEU:CD1	1:D:390:LEU:HB2	2.41	0.51
1:A:26:HIS:CE1	1:A:410:GLU:HG3	2.46	0.51
1:A:378:VAL:HG23	1:A:386:LEU:O	2.12	0.51
1:C:66:LEU:HG	1:C:67:GLY:N	2.26	0.51
1:C:142:ARG:NH2	4:C:616:HOH:O	2.30	0.51
1:A:66:LEU:HD12	1:A:101:PHE:O	2.11	0.51
1:D:379:GLN:O	1:D:379:GLN:HG3	2.11	0.51
1:A:198:TRP:CZ2	1:A:200:GLY:HA3	2.46	0.50
1:B:273:THR:HB	1:B:320:ASP:HB2	1.93	0.50
1:A:18:LEU:HB3	1:A:44:ILE:CG2	2.37	0.50
1:B:164:THR:O	1:B:165:LYS:CG	2.60	0.50
1:A:282:ASN:ND2	4:A:608:HOH:O	2.43	0.50
1:D:66:LEU:HD12	1:D:102:SER:HB3	1.92	0.50
1:B:378:VAL:HG23	1:B:386:LEU:O	2.12	0.50
1:C:126:ASN:OD1	1:C:129:VAL:N	2.44	0.50
1:B:13:SER:OG	1:B:49:SER:HA	2.12	0.50
1:B:201:ILE:HG23	1:B:202:GLU:H	1.75	0.50
1:B:320:ASP:OD2	1:B:334:SER:HB2	2.13	0.49
1:B:149:ASN:OD1	1:B:155:THR:OG1	2.26	0.49
1:D:18:LEU:O	1:D:43:PHE:HA	2.11	0.49
1:A:312:GLU:HB2	1:A:342:LEU:HB3	1.94	0.49
1:D:15:LEU:O	1:D:421:VAL:O	2.31	0.49
1:A:370:ARG:HB3	4:A:639:HOH:O	2.12	0.49
1:B:389:ARG:NE	1:B:391:ARG:HD2	2.26	0.49
1:D:347:VAL:HG11	1:D:357:TRP:O	2.12	0.49
1:A:139:GLN:HG3	1:A:140:THR:N	2.28	0.49
1:D:336:SER:OG	1:D:371:ASP:HB2	2.13	0.49
1:B:51:TYR:OH	1:B:109:LYS:HB3	2.12	0.49
1:D:26:HIS:HE1	1:D:410:GLU:OE2	1.95	0.49
1:B:369:GLU:HA	1:B:394:THR:O	2.12	0.49
1:B:66:LEU:HD23	1:B:68:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:OD1	1:A:223:ASP:C	2.52	0.49
1:C:384:LYS:O	1:C:385:ASP:HB2	2.13	0.49
1:D:404:VAL:CG1	1:D:405:ASP:N	2.76	0.48
1:B:26:HIS:NE2	1:B:410:GLU:OE2	2.32	0.48
1:C:59:GLY:C	1:C:109:LYS:HG2	2.34	0.48
1:B:18:LEU:HB3	1:B:44:ILE:CG2	2.39	0.48
1:B:23:TYR:CD1	1:B:413:VAL:HG13	2.41	0.48
1:D:155:THR:O	1:D:196:GLY:HA2	2.13	0.48
1:C:421:VAL:O	1:C:422:PHE:HB3	2.13	0.48
1:B:13:SER:HA	1:B:48:GLN:O	2.13	0.48
1:B:152:GLU:O	1:B:153:ASP:CG	2.52	0.48
1:D:41:GLN:O	1:D:67:GLY:HA2	2.13	0.47
1:B:67:GLY:CA	1:B:68:LEU:HD12	2.44	0.47
1:D:126:ASN:OD1	1:D:129:VAL:N	2.47	0.47
1:A:146:LEU:O	1:A:157:THR:HA	2.14	0.47
1:A:63:TYR:C	2:A:502:C8E:H52	2.34	0.47
1:A:13:SER:OG	1:A:49:SER:HA	2.15	0.47
1:B:144:VAL:HG21	2:B:503:C8E:H82	1.96	0.47
1:B:24:PHE:CD2	1:B:24:PHE:O	2.68	0.47
1:A:389:ARG:HE	1:A:391:ARG:HD2	1.80	0.47
1:D:273:THR:OG1	1:D:320:ASP:HB2	2.14	0.47
1:B:119:LEU:HD23	2:B:504:C8E:H42	1.96	0.47
1:C:374:LEU:CD1	1:C:390:LEU:HB2	2.45	0.47
1:B:246:VAL:HA	1:B:256:ILE:O	2.15	0.47
1:D:289:TYR:CE2	1:D:292:GLN:HA	2.50	0.47
1:B:316:LYS:HG2	1:B:317:LEU:N	2.30	0.47
1:C:164:THR:HG22	1:C:165:LYS:N	2.30	0.47
1:C:201:ILE:N	1:C:201:ILE:HD12	2.29	0.46
1:A:23:TYR:O	1:A:412:ARG:HA	2.15	0.46
1:D:201:ILE:CG2	1:D:202:GLU:H	2.20	0.46
1:D:45:ALA:O	1:D:63:TYR:HA	2.14	0.46
1:A:281:VAL:O	1:A:311:ASN:HA	2.15	0.46
1:D:148:ASN:HD21	1:D:150:SER:N	2.12	0.46
1:C:279:GLN:HB3	1:C:314:SER:OG	2.15	0.46
1:B:103:SER:CA	3:B:507:BOG:H1	2.45	0.46
1:D:154:LEU:O	1:D:154:LEU:HD13	2.16	0.46
1:B:153:ASP:C	1:B:153:ASP:OD1	2.53	0.46
1:D:128:VAL:HG21	1:D:211:ALA:HB2	1.97	0.46
1:B:195:GLY:HA3	1:B:209:TYR:CD2	2.51	0.46
1:D:366:LYS:HB2	1:D:398:THR:OG1	2.15	0.46
1:D:66:LEU:HG	1:D:67:GLY:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:VAL:O	1:A:385:ASP:N	2.34	0.46
1:C:19:THR:CG2	1:C:417:TYR:HB3	2.46	0.46
1:C:369:GLU:OE1	1:C:371:ASP:OD1	2.34	0.46
1:A:109:LYS:HA	1:A:117:LEU:O	2.15	0.46
1:A:143:GLY:HA2	2:A:504:C8E:H72	1.97	0.46
1:C:345:THR:HG23	1:C:362:GLY:O	2.16	0.46
1:A:49:SER:OG	1:A:60:VAL:N	2.42	0.46
1:D:137:LEU:HA	1:D:138:PRO:HD3	1.78	0.45
1:B:253:LEU:HA	1:B:253:LEU:HD23	1.72	0.45
1:A:396:ARG:HA	1:A:407:ASP:OD1	2.17	0.45
1:A:374:LEU:HD12	1:A:374:LEU:H	1.81	0.45
1:A:377:VAL:HG22	1:A:387:SER:HB2	1.96	0.45
1:D:148:ASN:HD21	1:D:150:SER:CB	2.20	0.45
1:C:378:VAL:HG11	1:C:383:ALA:CB	2.39	0.45
1:D:146:LEU:C	1:D:146:LEU:HD12	2.37	0.45
1:A:289:TYR:CD1	1:A:292:GLN:HG2	2.51	0.45
1:A:243:TYR:CG	1:A:287:PHE:CE1	3.04	0.45
1:A:254:GLY:HA3	1:A:352:PRO:HD2	1.98	0.45
1:A:152:GLU:O	1:A:153:ASP:HB3	2.15	0.45
1:A:421:VAL:O	1:A:422:PHE:C	2.55	0.45
1:A:126:ASN:HB2	1:A:127:PRO:CD	2.47	0.45
1:A:128:VAL:HG21	1:A:211:ALA:HB2	1.99	0.45
1:B:303:GLN:HE21	1:B:410:GLU:HG2	1.82	0.45
1:C:281:VAL:O	1:C:311:ASN:HA	2.17	0.45
1:D:17:LEU:HB3	1:D:419:ILE:HB	1.99	0.45
1:A:226:TYR:HB3	1:A:238:PRO:HG2	1.99	0.44
1:C:137:LEU:HA	1:C:138:PRO:HD3	1.82	0.44
1:C:164:THR:HG22	1:C:165:LYS:H	1.81	0.44
1:B:191:LEU:HA	1:B:212:GLU:O	2.18	0.44
1:A:384:LYS:HE3	1:A:385:ASP:OD2	2.17	0.44
1:C:39:TRP:HE1	1:C:70:LEU:HD12	1.81	0.44
1:B:146:LEU:HD13	1:B:147:THR:N	2.32	0.44
1:B:289:TYR:CZ	1:B:292:GLN:HG2	2.53	0.44
1:A:23:TYR:HB3	1:A:413:VAL:HG13	1.99	0.44
1:A:187:ASP:CG	1:A:188:SER:N	2.70	0.44
1:B:226:TYR:HB3	1:B:238:PRO:HG2	1.99	0.44
1:C:211:ALA:C	2:C:502:C8E:H111	2.38	0.44
1:A:279:GLN:HB3	1:A:314:SER:OG	2.17	0.44
1:A:253:LEU:HD22	1:A:353:GLY:HA3	1.99	0.44
1:D:17:LEU:CD1	1:D:43:PHE:CD2	3.01	0.44
1:C:404:VAL:CG1	1:C:405:ASP:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LYS:HE2	1:B:188:SER:HA	2.00	0.44
1:D:26:HIS:ND1	1:D:410:GLU:HB2	2.33	0.44
1:D:397:GLY:HA3	1:D:401:TYR:HB3	1.99	0.44
1:A:408:ILE:H	1:A:408:ILE:HD13	1.82	0.43
1:D:142:ARG:NH1	2:D:501:C8E:C1	2.81	0.43
1:B:204:PHE:HA	1:B:225:ASP:O	2.17	0.43
1:C:18:LEU:O	1:C:43:PHE:HA	2.18	0.43
1:C:259:ASN:O	1:C:282:ASN:HB2	2.18	0.43
1:C:11:GLU:H	1:C:11:GLU:CD	2.18	0.43
2:B:503:C8E:H71	2:B:503:C8E:H101	1.53	0.43
1:B:410:GLU:OE1	1:B:412:ARG:NE	2.52	0.43
1:B:154:LEU:HD23	1:B:154:LEU:HA	1.81	0.43
1:D:59:GLY:C	1:D:109:LYS:HG2	2.39	0.43
1:D:390:LEU:HD12	1:D:413:VAL:HG23	2.01	0.43
1:B:395:HIS:C	1:B:396:ARG:HD2	2.39	0.43
1:D:43:PHE:HE2	1:D:45:ALA:HB2	1.83	0.43
1:B:127:PRO:HG3	1:B:297:PHE:CE2	2.53	0.43
1:C:65:MET:HB3	1:C:65:MET:HE2	1.59	0.43
1:D:384:LYS:O	1:D:385:ASP:HB2	2.18	0.43
1:B:320:ASP:OD2	1:B:334:SER:CB	2.67	0.43
1:C:201:ILE:CD1	1:C:201:ILE:N	2.82	0.43
1:C:108:LEU:HD22	1:C:109:LYS:H	1.84	0.43
1:D:127:PRO:HA	1:D:297:PHE:CD1	2.54	0.43
1:C:12:GLY:HA3	1:C:50:GLY:HA3	2.01	0.43
1:A:363:LYS:HA	1:A:363:LYS:HD3	1.55	0.43
1:C:17:LEU:HD11	1:C:43:PHE:CD1	2.54	0.42
1:A:108:LEU:HD22	1:A:109:LYS:N	2.34	0.42
1:A:298:LEU:HA	1:A:298:LEU:HD23	1.83	0.42
1:A:331:LEU:HB2	1:A:376:TYR:HD1	1.84	0.42
1:B:152:GLU:O	1:B:153:ASP:CB	2.68	0.42
1:A:162:SER:HA	1:A:189:HIS:O	2.18	0.42
1:A:302:GLN:O	1:A:303:GLN:C	2.56	0.42
1:A:39:TRP:CD1	1:A:70:LEU:HB2	2.54	0.42
1:C:108:LEU:HD22	1:C:109:LYS:N	2.34	0.42
1:B:126:ASN:HB2	1:B:127:PRO:CD	2.49	0.42
1:B:65:MET:O	1:B:102:SER:HA	2.19	0.42
1:C:119:LEU:HD12	1:C:119:LEU:N	2.33	0.42
1:A:395:HIS:O	1:A:396:ARG:HD2	2.20	0.42
1:C:139:GLN:CG	1:C:140:THR:N	2.82	0.42
1:B:363:LYS:HB3	1:B:364:ASN:H	1.71	0.42
1:C:126:ASN:HB2	1:C:127:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HA	1:A:212:GLU:O	2.19	0.42
1:A:10:ILE:O	1:A:13:SER:HB2	2.19	0.42
1:A:195:GLY:HA3	1:A:209:TYR:CD2	2.55	0.42
1:C:348:ASP:OD1	1:C:350:ASP:N	2.46	0.42
1:A:154:LEU:HD11	2:C:502:C8E:H21	2.01	0.42
1:A:126:ASN:HB2	1:A:127:PRO:HD2	2.01	0.42
1:D:124:LEU:HD12	1:D:141:PHE:CD2	2.55	0.42
1:A:221:TYR:C	1:A:221:TYR:CD2	2.92	0.42
1:C:17:LEU:HD11	1:C:43:PHE:CE1	2.55	0.42
1:D:126:ASN:HB2	1:D:127:PRO:CD	2.49	0.42
1:A:368:TRP:O	1:A:395:HIS:HA	2.19	0.42
1:A:13:SER:HA	1:A:48:GLN:O	2.20	0.41
1:C:217:TRP:C	1:C:217:TRP:CD1	2.93	0.41
1:D:207:SER:O	1:D:222:ALA:HA	2.20	0.41
1:B:201:ILE:HB	1:B:204:PHE:HD2	1.85	0.41
1:D:43:PHE:CD2	1:D:43:PHE:C	2.94	0.41
1:D:154:LEU:HA	1:D:197:THR:O	2.20	0.41
1:B:198:TRP:CE2	1:B:200:GLY:HA3	2.54	0.41
1:D:23:TYR:HB2	1:D:39:TRP:CZ3	2.56	0.41
1:A:237:ASN:HA	1:A:238:PRO:HD2	1.95	0.41
1:A:364:ASN:O	1:A:366:LYS:HG3	2.20	0.41
1:A:221:TYR:HA	1:A:242:TYR:O	2.21	0.41
1:B:239:GLY:HA3	1:B:264:HIS:CE1	2.55	0.41
1:C:134:SER:HB2	1:C:135:ARG:HG2	2.00	0.41
1:D:44:ILE:HD12	1:D:45:ALA:N	2.35	0.41
2:B:503:C8E:H102	2:B:503:C8E:H132	1.86	0.41
1:B:113:PHE:HB2	2:B:502:C8E:H142	2.02	0.41
1:B:201:ILE:CG2	1:B:204:PHE:H	2.34	0.41
1:A:362:GLY:O	1:A:364:ASN:N	2.53	0.41
1:B:104:GLY:N	3:B:507:BOG:C2	2.83	0.41
1:B:154:LEU:HD22	1:B:155:THR:N	2.35	0.41
1:A:389:ARG:NE	1:A:391:ARG:HD2	2.36	0.41
1:C:296:ILE:HG22	1:C:297:PHE:CD2	2.55	0.41
1:A:246:VAL:HA	1:A:256:ILE:O	2.19	0.41
1:A:23:TYR:HB2	1:A:39:TRP:CE3	2.56	0.41
1:A:164:THR:O	1:A:165:LYS:CD	2.68	0.41
1:C:231:ASP:CB	1:C:233:ASN:H	2.34	0.41
1:A:204:PHE:HA	1:A:225:ASP:O	2.21	0.41
1:A:23:TYR:CD2	1:A:413:VAL:HG13	2.55	0.41
1:B:303:GLN:NE2	1:B:410:GLU:HG2	2.36	0.41
1:C:44:ILE:HD12	1:C:45:ALA:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:TYR:CD1	1:B:292:GLN:HG2	2.55	0.41
1:B:396:ARG:HB2	4:B:610:HOH:O	2.21	0.41
1:A:139:GLN:OE1	1:A:166:TYR:CD1	2.74	0.41
1:B:422:PHE:CD1	1:B:422:PHE:C	2.94	0.41
1:D:374:LEU:HD12	1:D:390:LEU:HB2	2.03	0.41
1:A:322:ASP:OD1	1:A:324:VAL:HG23	2.21	0.41
1:B:24:PHE:HA	1:B:411:TYR:O	2.21	0.40
1:D:51:TYR:CZ	1:D:109:LYS:HE3	2.56	0.40
1:B:223:ASP:OD1	1:B:223:ASP:C	2.60	0.40
1:D:217:TRP:C	1:D:217:TRP:CD1	2.94	0.40
1:A:15:LEU:O	1:A:421:VAL:HG13	2.21	0.40
1:C:146:LEU:HD12	1:C:146:LEU:C	2.41	0.40
1:D:227:THR:HG22	1:D:227:THR:O	2.20	0.40
1:C:204:PHE:HA	1:C:225:ASP:O	2.22	0.40
1:B:395:HIS:HB3	1:B:408:ILE:HD11	2.01	0.40
1:A:374:LEU:HD12	1:A:374:LEU:N	2.37	0.40
1:C:380:GLY:HA2	1:C:384:LYS:HG3	2.02	0.40
1:B:15:LEU:HD12	1:B:46:THR:O	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	361/430 (84%)	341 (94%)	19 (5%)	1 (0%)	46	79
1	B	362/430 (84%)	338 (93%)	23 (6%)	1 (0%)	46	79
1	C	350/430 (81%)	335 (96%)	15 (4%)	0	100	100
1	D	353/430 (82%)	338 (96%)	14 (4%)	1 (0%)	46	79
All	All	1426/1720 (83%)	1352 (95%)	71 (5%)	3 (0%)	52	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	363	LYS
1	A	363	LYS
1	D	152	GLU

### 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	291/349 (83%)	252 (87%)	39 (13%)	5	14
1	B	292/349 (84%)	252 (86%)	40 (14%)	4	13
1	C	275/349 (79%)	233 (85%)	42 (15%)	3	10
1	D	278/349 (80%)	234 (84%)	44 (16%)	3	9
All	All	1136/1396 (81%)	971 (86%)	165 (14%)	4	11

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	26	HIS
1	A	27	ASP
1	A	29	ARG
1	A	46	THR
1	A	65	MET
1	A	99	ASP
1	A	108	LEU
1	A	119	LEU
1	A	129	VAL
1	A	134	SER
1	A	142	ARG
1	A	146	LEU
1	A	152	GLU
1	A	153	ASP
1	A	154	LEU
1	A	166	TYR
1	A	188	SER
1	A	192	SER

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Mol	Chain	Res	Type
1	A	204	PHE
1	A	206	SER
1	A	208	LEU
1	A	228	TYR
1	A	229	GLU
1	A	233	ASN
1	A	262	SER
1	A	273	THR
1	A	275	THR
1	A	278	LEU
1	A	313	LYS
1	A	328	VAL
1	A	363	LYS
1	A	367	HIS
1	A	374	LEU
1	A	390	LEU
1	A	396	ARG
1	A	404	VAL
1	A	408	ILE
1	A	422	PHE
1	B	24	PHE
1	B	26	HIS
1	B	44	ILE
1	B	46	THR
1	B	65	MET
1	B	66	LEU
1	B	68	LEU
1	B	99	ASP
1	B	108	LEU
1	B	129	VAL
1	B	146	LEU
1	B	153	ASP
1	B	154	LEU
1	B	165	LYS
1	B	166	TYR
1	B	187	ASP
1	B	201	ILE
1	B	206	SER
1	B	208	LEU
1	B	217	TRP
1	B	226	TYR
1	B	228	TYR

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Mol	Chain	Res	Type
1	B	230	ILE
1	B	232	ASP
1	B	255	ARG
1	B	275	THR
1	B	278	LEU
1	B	328	VAL
1	B	336	SER
1	B	339	ARG
1	B	341	LYS
1	B	363	LYS
1	B	367	HIS
1	B	370	ARG
1	B	374	LEU
1	B	390	LEU
1	B	396	ARG
1	B	408	ILE
1	B	421	VAL
1	B	422	PHE
1	C	19	THR
1	C	20	ARG
1	C	21	ASN
1	C	26	HIS
1	C	43	PHE
1	C	44	ILE
1	C	46	THR
1	C	65	MET
1	C	108	LEU
1	C	125	SER
1	C	129	VAL
1	C	134	SER
1	C	135	ARG
1	C	145	SER
1	C	146	LEU
1	C	151	PHE
1	C	154	LEU
1	C	188	SER
1	C	189	HIS
1	C	193	TRP
1	C	198	TRP
1	C	205	THR
1	C	206	SER
1	C	208	LEU

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Mol	Chain	Res	Type
1	C	227	THR
1	C	273	THR
1	C	282	ASN
1	C	296	ILE
1	C	326	LEU
1	C	328	VAL
1	C	336	SER
1	C	342	LEU
1	C	359	SER
1	C	367	HIS
1	C	374	LEU
1	C	387	SER
1	C	390	LEU
1	C	402	SER
1	C	404	VAL
1	C	408	ILE
1	C	413	VAL
1	C	421	VAL
1	D	17	LEU
1	D	19	THR
1	D	20	ARG
1	D	21	ASN
1	D	26	HIS
1	D	43	PHE
1	D	44	ILE
1	D	108	LEU
1	D	119	LEU
1	D	129	VAL
1	D	134	SER
1	D	146	LEU
1	D	148	ASN
1	D	150	SER
1	D	154	LEU
1	D	188	SER
1	D	193	TRP
1	D	205	THR
1	D	206	SER
1	D	227	THR
1	D	245	THR
1	D	255	ARG
1	D	273	THR
1	D	282	ASN

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Mol	Chain	Res	Type
1	D	328	VAL
1	D	342	LEU
1	D	359	SER
1	D	367	HIS
1	D	370	ARG
1	D	372	LEU
1	D	374	LEU
1	D	379	GLN
1	D	387	SER
1	D	389	ARG
1	D	390	LEU
1	D	396	ARG
1	D	402	SER
1	D	404	VAL
1	D	408	ILE
1	D	409	ASP
1	D	410	GLU
1	D	413	VAL
1	D	420	ASP
1	D	421	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	139	GLN
1	C	139	GLN
1	C	148	ASN
1	C	303	GLN
1	D	26	HIS
1	D	148	ASN
1	D	282	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 ⓘ

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	C8E	A	501	-	13,13,20	0.58	0	12,12,19	0.46	0
2	C8E	A	502	-	11,11,20	0.32	0	10,10,19	0.58	0
2	C8E	A	503	-	15,15,20	0.49	0	14,14,19	0.54	0
2	C8E	A	504	-	15,15,20	0.43	0	14,14,19	0.32	0
2	C8E	A	505	-	20,20,20	0.47	0	19,19,19	0.41	0
3	BOG	A	506	-	16,16,20	1.31	2 (12%)	21,21,25	2.21	8 (38%)
2	C8E	B	501	-	9,9,20	0.33	0	8,8,19	0.75	0
2	C8E	B	502	-	15,15,20	0.55	0	14,14,19	0.53	0
2	C8E	B	503	-	14,14,20	0.40	0	13,13,19	0.49	0
2	C8E	B	504	-	15,15,20	0.39	0	14,14,19	0.52	0
2	C8E	B	505	-	20,20,20	0.43	0	19,19,19	0.46	0
2	C8E	B	506	-	10,10,20	0.41	0	9,9,19	0.40	0
3	BOG	B	507	-	15,15,20	1.50	3 (20%)	20,20,25	2.65	10 (50%)
2	C8E	C	501	-	8,8,20	0.50	0	7,7,19	0.30	0
2	C8E	C	502	-	15,15,20	0.44	0	14,14,19	0.30	0
2	C8E	C	503	-	17,17,20	0.49	0	16,16,19	0.34	0
2	C8E	C	504	-	10,10,20	0.41	0	9,9,19	0.44	0
2	C8E	C	505	-	7,7,20	0.35	0	6,6,19	0.37	0
2	C8E	D	501	-	9,9,20	0.34	0	8,8,19	0.51	0
2	C8E	D	502	-	11,11,20	0.57	0	10,10,19	0.34	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	C8E	A	501	-	-	0/11/11/18	0/0/0/0
2	C8E	A	502	-	-	0/9/9/18	0/0/0/0
2	C8E	A	503	-	-	0/13/13/18	0/0/0/0
2	C8E	A	504	-	-	0/13/13/18	0/0/0/0
2	C8E	A	505	-	-	0/18/18/18	0/0/0/0
3	BOG	A	506	-	2/2/5/5	0/7/27/31	0/1/1/1
2	C8E	B	501	-	-	0/7/7/18	0/0/0/0
2	C8E	B	502	-	-	0/13/13/18	0/0/0/0
2	C8E	B	503	-	-	0/12/12/18	0/0/0/0
2	C8E	B	504	-	-	0/13/13/18	0/0/0/0
2	C8E	B	505	-	-	0/18/18/18	0/0/0/0
2	C8E	B	506	-	-	0/8/8/18	0/0/0/0
3	BOG	B	507	-	2/2/5/5	0/6/26/31	0/1/1/1
2	C8E	C	501	-	-	0/6/6/18	0/0/0/0
2	C8E	C	502	-	-	0/13/13/18	0/0/0/0
2	C8E	C	503	-	-	0/15/15/18	0/0/0/0
2	C8E	C	504	-	-	0/8/8/18	0/0/0/0
2	C8E	C	505	-	-	0/5/5/18	0/0/0/0
2	C8E	D	501	-	-	0/7/7/18	0/0/0/0
2	C8E	D	502	-	-	0/9/9/18	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	507	BOG	C4-C3	-3.78	1.42	1.52
3	A	506	BOG	C4-C3	-3.48	1.43	1.52
3	B	507	BOG	C3-C2	-2.04	1.47	1.52
3	A	506	BOG	O3-C3	2.26	1.48	1.43
3	B	507	BOG	O3-C3	2.49	1.48	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	507	BOG	O2-C2-C3	-2.50	104.72	110.34
3	B	507	BOG	O3-C3-C2	-2.30	105.16	110.34
3	A	506	BOG	O6-C6-C5	2.05	118.11	111.33
3	A	506	BOG	C1-O5-C5	2.35	118.30	113.75
3	B	507	BOG	C4-C3-C2	2.42	115.30	110.79
3	A	506	BOG	C1-C2-C3	2.45	114.80	109.97
3	B	507	BOG	C1-O5-C5	2.46	118.53	113.75
3	A	506	BOG	O1-C1-C2	2.77	111.54	108.04
3	B	507	BOG	O5-C1-C2	2.93	116.29	110.28
3	A	506	BOG	C1'-O1-C1	3.30	119.71	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	506	BOG	O5-C1-C2	3.49	117.44	110.28
3	B	507	BOG	O1-C1'-C2'	3.63	120.36	109.96
3	B	507	BOG	C3-C4-C5	4.10	117.35	110.20
3	B	507	BOG	C1-C2-C3	4.31	118.47	109.97
3	B	507	BOG	O5-C5-C4	4.32	117.78	109.68
3	A	506	BOG	C3-C4-C5	4.53	118.09	110.20
3	A	506	BOG	O5-C5-C4	4.63	118.37	109.68
3	B	507	BOG	C1'-O1-C1	5.46	123.48	113.94

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	506	BOG	C5
3	A	506	BOG	C3
3	B	507	BOG	C5
3	B	507	BOG	C3

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	C8E	1	0
2	A	504	C8E	1	0
3	A	506	BOG	2	0
2	B	502	C8E	1	0
2	B	503	C8E	3	0
2	B	504	C8E	1	0
3	B	507	BOG	6	0
2	C	502	C8E	2	0
2	D	501	C8E	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	371/430 (86%)	-0.28	2 (0%) 91 88	41, 63, 111, 145	0
1	B	372/430 (86%)	-0.35	1 (0%) 94 92	38, 64, 109, 136	0
1	C	360/430 (83%)	-0.37	0 100 100	38, 71, 111, 135	0
1	D	361/430 (83%)	-0.34	0 100 100	38, 70, 111, 130	0
All	All	1464/1720 (85%)	-0.33	3 (0%) 95 94	38, 67, 111, 145	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	327	GLY	3.8
1	B	228	TYR	2.3
1	A	228	TYR	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	C8E	A	501	14/21	0.77	0.37	5.45	49,82,90,90	0
2	C8E	B	503	15/21	0.88	0.33	4.62	53,69,107,108	0
2	C8E	B	506	11/21	0.90	0.30	4.60	54,67,88,91	0
2	C8E	A	505	21/21	0.85	0.30	4.52	42,67,94,98	0
2	C8E	A	503	16/21	0.83	0.33	4.12	65,73,84,90	0
2	C8E	C	503	18/21	0.67	0.27	4.06	82,99,113,114	0
2	C8E	A	502	12/21	0.92	0.24	3.52	58,65,68,71	0
2	C8E	B	505	21/21	0.94	0.30	3.36	52,79,90,93	0
2	C8E	A	504	16/21	0.87	0.33	3.12	60,79,91,91	0
2	C8E	B	504	16/21	0.93	0.24	2.92	60,73,101,104	0
2	C8E	B	502	16/21	0.92	0.25	2.71	51,71,90,93	0
2	C8E	C	502	16/21	0.91	0.25	2.25	55,75,95,96	0
2	C8E	C	501	9/21	0.91	0.24	1.96	67,78,85,85	0
2	C8E	C	504	11/21	0.85	0.28	1.60	54,67,101,102	0
2	C8E	C	505	8/21	0.86	0.24	1.19	60,68,84,88	0
2	C8E	D	502	12/21	0.90	0.22	1.12	60,74,97,100	0
2	C8E	B	501	10/21	0.89	0.20	0.88	52,61,72,72	0
2	C8E	D	501	10/21	0.94	0.22	0.87	69,76,79,79	0
3	BOG	A	506	16/20	0.90	0.16	0.34	67,81,93,104	0
3	BOG	B	507	15/20	0.84	0.15	-0.14	49,92,113,116	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.