

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 2, 2023 – 03:02 AM EDT

PDB ID	:	1BXN
Title	:	THE CRYSTAL STRUCTURE OF RUBISCO FROM ALCALIGENES EU-
		TROPHUS TO 2.7 ANGSTROMS.
Authors	:	Hansen, S.; Vollan, V.B.; Hough, E.; Andersen, K.
Deposited on	:	1998-10-06
Resolution	:	2.70  Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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	:	2.34
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)	:	2.34

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 2.70 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)	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range({\rm \AA})}) \end{array}$
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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.

Mol	Chain	Length	Quality of chain					
1	А	485	65%	24%	• 8%			
1	С	485	9%	24%	• 8%			
1	Е	485	65%	24%	• 8%			
1	G	485	8%	23%	• 8%			
2	Ι	139	10%	33%	5% 7%			
2	J	139	53%	35%	5% 7%			
2	К	139	10%	35%	• 7%			



Mol	Chain	Length	Quality	of chain	
_	-		12%		
2	L	139	50%	37%	5% 7%



#### $1\mathrm{BXN}$

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18144 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 PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	445	Total	С	Ν	Ο	S	0	0	0
1	Л	440	3470	2201	612	636	21	0	0	U
1	С	445	Total	С	Ν	0	S	0	0	0
1	U	440	3470	2201	612	636	21	0	0	0
1	F	445	Total	С	Ν	0	S	0	0	0
1	Ľ	440	3470	2201	612	636	21			
1	1 C	0 445	Total	С	Ν	0	S	0	0	0
I G	445	3470	2201	612	636	21	U	U	0	

• Molecule 2 is a protein called PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	Т	120	Total	С	Ν	0	S	0	0	0
	1	129	1056	670	180	200	6	0	0	0
9	т	120	Total	С	Ν	Ο	S	0	0	0
	J	129	1056	670	180	200	6	0	0	0
0	K	120	Total	С	Ν	0	S	0	0	0
	Γ	129	1056	670	180	200	6	0	0	0
0	9 I	120	Total	С	Ν	0	S	0	0	0
	L	129	1056	670	180	200	6	0	0	U

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	Ε	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0



# 3 Residue-property plots (i)

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: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN)







# F788 1100 1100 1100 1100 1100 1100 1100 1100 1111 1111 1111 1111 1111 1111 1111 1112 1112 1112 1112 1112 1112 1112 1112 1112 1112 1112 1112 1112 1112 1112 1112 1112 1120 1121 1122 1123 1124 1123 1124 1120 1121 1122 1123 1124 1125 1120 1121 1122 1123

• Molecule 2: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN)



• Molecule 2: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN)



• Molecule 2: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN)





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	112.00Å 112.00Å 402.70Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	15.00 - 2.70	Depositor
Resolution (A)	24.60 - 2.65	EDS
% Data completeness	90.0 (15.00-2.70)	Depositor
(in resolution range)	86.9 (24.60-2.65)	EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.12 (at 2.64 \text{\AA})$	Xtriage
Refinement program	X-PLOR 3.8	Depositor
P. P.	0.266 , $0.322$	Depositor
$n, n_{free}$	0.280 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	45.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29, $50.0$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	18144	wwPDB-VP
Average B, all atoms $(Å^2)$	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: PO4

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).

Mal	Mol Chain		lengths	Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.33	0/3552	0.57	0/4816	
1	С	0.33	0/3552	0.57	0/4816	
1	Е	0.33	0/3552	0.57	0/4816	
1	G	0.34	0/3552	0.57	0/4816	
2	Ι	0.37	0/1084	0.61	0/1474	
2	J	0.36	0/1084	0.61	0/1474	
2	Κ	0.36	0/1084	0.61	0/1474	
2	L	0.36	0/1084	0.61	0/1474	
All	All	0.34	0/18544	0.58	0/25160	

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	А	3470	0	3402	89	0
1	С	3470	0	3402	88	0
1	Е	3470	0	3402	86	0
1	G	3470	0	3402	84	0
2	Ι	1056	0	1007	37	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1056	0	1007	39	0
2	Κ	1056	0	1007	39	0
2	L	1056	0	1007	42	0
3	А	10	0	0	0	0
3	С	10	0	0	0	0
3	Е	10	0	0	0	0
3	G	10	0	0	1	0
All	All	18144	0	17636	467	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 13.

All (467) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:420:THR:HG23	2:I:10:PHE:HE2	1.48	0.79
1:G:433:ARG:HH21	1:G:434:ASN:HD21	1.31	0.78
1:C:420:THR:HG23	2:J:10:PHE:HE2	1.50	0.77
1:C:433:ARG:HH21	1:C:434:ASN:HD21	1.32	0.77
1:E:433:ARG:HH21	1:E:434:ASN:HD21	1.29	0.77
2:J:38:THR:HG22	2:J:40:ASP:H	1.51	0.76
1:A:433:ARG:HH21	1:A:434:ASN:HD21	1.30	0.76
2:K:38:THR:HG22	2:K:40:ASP:H	1.52	0.75
1:A:245:VAL:HG21	1:A:268:ILE:HD11	1.69	0.74
1:E:420:THR:HG23	2:K:10:PHE:HE2	1.51	0.74
2:I:38:THR:HG22	2:I:40:ASP:H	1.52	0.74
2:J:112:VAL:HB	2:J:124:SER:HB2	1.70	0.74
2:K:112:VAL:HB	2:K:124:SER:HB2	1.69	0.74
2:L:38:THR:HG22	2:L:40:ASP:H	1.51	0.73
1:C:245:VAL:HG21	1:C:268:ILE:HD11	1.71	0.73
2:K:104:ALA:O	2:K:107:PRO:HD3	1.89	0.73
1:G:245:VAL:HG21	1:G:268:ILE:HD11	1.69	0.72
1:G:420:THR:HG23	2:L:10:PHE:HE2	1.54	0.72
2:L:83:THR:HG22	2:L:95:VAL:HG22	1.70	0.72
1:G:158:ILE:HG12	1:G:377:MET:HG2	1.72	0.72
1:C:158:ILE:HG12	1:C:377:MET:HG2	1.70	0.72
2:L:55:MET:HG3	2:L:64:ILE:HG12	1.72	0.72
2:L:104:ALA:O	2:L:107:PRO:HD3	1.89	0.72
2:J:104:ALA:O	2:J:107:PRO:HD3	1.90	0.72
2:I:112:VAL:HB	2:I:124:SER:HB2	1.72	0.71
1:E:245:VAL:HG21	1:E:268:ILE:HD11	1.71	0.71



	lo uo pugo	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:J:83:THR:HG22	2:J:95:VAL:HG22	1.72	0.71
2:I:55:MET:HG3	2:I:64:ILE:HG12	1.71	0.71
1:A:158:ILE:HG12	1:A:377:MET:HG2	1.73	0.71
2:K:83:THR:HG22	2:K:95:VAL:HG22	1.73	0.70
2:K:25:TYR:O	2:K:29:GLN:HG2	1.91	0.70
2:L:112:VAL:HB	2:L:124:SER:HB2	1.72	0.70
2:I:83:THR:HG22	2:I:95:VAL:HG22	1.71	0.70
1:G:332:THR:HG21	1:G:336:LYS:HB3	1.74	0.70
1:A:297:ARG:HG2	1:A:329:HIS:HB2	1.74	0.69
2:I:104:ALA:O	2:I:107:PRO:HD3	1.91	0.69
1:G:297:ARG:HG2	1:G:329:HIS:HB2	1.74	0.69
2:I:25:TYR:O	2:I:29:GLN:HG2	1.93	0.69
1:E:332:THR:HG21	1:E:336:LYS:HB3	1.74	0.69
2:K:55:MET:HG3	2:K:64:ILE:HG12	1.75	0.69
1:C:297:ARG:HG2	1:C:329:HIS:HB2	1.75	0.69
1:A:332:THR:HG21	1:A:336:LYS:HB3	1.74	0.68
1:C:332:THR:HG21	1:C:336:LYS:HB3	1.75	0.68
2:J:47:TYR:HA	1:E:190:ARG:NH2	2.08	0.68
1:E:158:ILE:HG12	1:E:377:MET:HG2	1.73	0.68
1:E:297:ARG:HG2	1:E:329:HIS:HB2	1.76	0.68
2:J:55:MET:HG3	2:J:64:ILE:HG12	1.75	0.68
2:J:25:TYR:O	2:J:29:GLN:HG2	1.93	0.67
1:E:179:PRO:HB3	1:E:183:LEU:HD13	1.77	0.67
1:A:179:PRO:HB3	1:A:183:LEU:HD13	1.76	0.67
2:L:25:TYR:O	2:L:29:GLN:HG2	1.94	0.67
1:G:179:PRO:HB3	1:G:183:LEU:HD13	1.77	0.66
1:A:183:LEU:HA	2:L:90:THR:HB	1.78	0.66
1:G:62:GLY:O	1:G:67:ALA:HB3	1.96	0.66
1:E:62:GLY:O	1:E:67:ALA:HB3	1.96	0.65
1:A:62:GLY:O	1:A:67:ALA:HB3	1.96	0.65
1:E:242:TYR:HB3	1:E:269:MET:HB2	1.78	0.65
1:C:179:PRO:HB3	1:C:183:LEU:HD13	1.77	0.64
1:C:242:TYR:HB3	1:C:269:MET:HB2	1.79	0.64
1:C:62:GLY:O	1:C:67:ALA:HB3	1.98	0.64
1:A:420:THR:HG23	2:I:10:PHE:CE2	2.32	0.63
1:A:242:TYR:HB3	1:A:269:MET:HB2	1.81	0.63
1:A:180:LYS:HG2	1:A:181:LEU:H	1.64	0.63
1:C:334:VAL:HB	1:C:341:PRO:HG3	1.82	0.62
1:G:242:TYR:HB3	1:G:269:MET:HB2	1.82	0.61
1:E:180:LYS:HG2	1:E:181:LEU:H	1.66	0.61
$1:\overline{G:274:VAL:HG12}$	1:G:278:CYS:CB	2.30	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:334:VAL:HB	1:E:341:PRO:HG3	1.83	0.61
2:K:90:THR:HB	1:G:183:LEU:HA	1.83	0.60
1:A:274:VAL:HG12	1:A:278:CYS:CB	2.30	0.60
1:G:334:VAL:HB	1:G:341:PRO:HG3	1.83	0.60
1:G:180:LYS:HG2	1:G:181:LEU:H	1.65	0.60
1:C:180:LYS:HG2	1:C:181:LEU:H	1.67	0.59
1:C:274:VAL:HG12	1:C:278:CYS:CB	2.31	0.59
2:L:44:ARG:HH11	2:L:44:ARG:HA	1.67	0.59
1:C:136:ALA:O	1:C:309:HIS:HA	2.03	0.59
1:A:334:VAL:HB	1:A:341:PRO:HG3	1.84	0.59
1:A:145:VAL:HG13	1:A:371:ALA:HB2	1.85	0.59
1:E:274:VAL:HG12	1:E:278:CYS:CB	2.32	0.59
1:E:61:ALA:HB1	1:E:85:ALA:O	2.03	0.59
2:J:44:ARG:HH11	2:J:44:ARG:HA	1.69	0.58
1:G:61:ALA:HB1	1:G:85:ALA:O	2.03	0.58
1:A:433:ARG:HG3	1:A:439:ILE:HD11	1.86	0.58
1:C:61:ALA:HB1	1:C:85:ALA:O	2.04	0.58
1:C:333:ALA:HB2	1:C:344:VAL:HG11	1.86	0.58
2:K:44:ARG:HA	2:K:44:ARG:HH11	1.66	0.58
1:E:433:ARG:HG3	1:E:439:ILE:HD11	1.85	0.58
1:G:245:VAL:HG22	1:G:256:ARG:HB2	1.84	0.58
1:E:68:THR:HG23	1:E:70:THR:O	2.04	0.57
1:C:420:THR:HG23	2:J:10:PHE:CE2	2.34	0.57
1:C:433:ARG:HG3	1:C:439:ILE:HD11	1.85	0.57
1:A:433:ARG:HH21	1:A:434:ASN:ND2	2.00	0.57
2:K:15:THR:H	2:K:18:GLN:HE21	1.52	0.57
1:A:189:GLY:HA3	2:L:47:TYR:OH	2.05	0.57
1:A:333:ALA:HB2	1:A:344:VAL:HG11	1.87	0.57
2:J:90:THR:HB	1:E:183:LEU:HA	1.87	0.57
1:A:61:ALA:HB1	1:A:85:ALA:O	2.04	0.57
2:I:15:THR:H	2:I:18:GLN:HE21	1.52	0.57
1:A:68:THR:HG23	1:A:70:THR:O	2.05	0.57
1:A:433:ARG:NH2	1:A:434:ASN:HD21	2.02	0.57
1:C:68:THR:HG23	1:C:70:THR:O	2.05	0.57
2:I:44:ARG:HA	2:I:44:ARG:HH11	1.68	0.57
1:C:145:VAL:HG13	1:C:371:ALA:HB2	1.85	0.57
2:J:15:THR:H	2:J:18:GLN:HE21	1.53	0.57
1:E:245:VAL:HG22	1:E:256:ARG:HB2	1.87	0.57
1:E:23:LYS:HA	1:E:58:ALA:HB1	1.87	0.56
1:E:433:ARG:HH21	1:E:434:ASN:ND2	2.00	0.56
1:G:336:LYS:HG3	1:G:383:GLY:H	1.70	0.56



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:G:136:ALA:O	1:G:309:HIS:HA	2.05	0.56
1:C:336:LYS:HG3	1:C:383:GLY:H	1.70	0.56
1:E:136:ALA:O	1:E:309:HIS:HA	2.05	0.56
1:E:145:VAL:HG13	1:E:371:ALA:HB2	1.86	0.56
1:E:179:PRO:HG2	1:E:191:VAL:HG21	1.88	0.56
1:G:274:VAL:HG12	1:G:278:CYS:HB2	1.88	0.56
1:G:433:ARG:HG3	1:G:439:ILE:HD11	1.86	0.56
1:G:68:THR:HG23	1:G:70:THR:O	2.05	0.56
1:G:145:VAL:HG13	1:G:371:ALA:HB2	1.87	0.56
1:A:23:LYS:HA	1:A:58:ALA:HB1	1.86	0.56
1:E:420:THR:HG23	2:K:10:PHE:CE2	2.36	0.56
1:E:433:ARG:NH2	1:E:434:ASN:HD21	2.02	0.56
1:A:336:LYS:HG3	1:A:383:GLY:H	1.70	0.56
2:I:90:THR:HB	1:C:183:LEU:HA	1.88	0.56
1:G:23:LYS:HA	1:G:58:ALA:HB1	1.87	0.56
1:A:337:LEU:H	1:A:337:LEU:HD22	1.71	0.55
1:G:433:ARG:NH2	1:G:434:ASN:HD21	2.02	0.55
1:E:336:LYS:HG3	1:E:383:GLY:H	1.70	0.55
1:C:433:ARG:NH2	1:C:434:ASN:HD21	2.04	0.55
2:J:82:VAL:HG23	2:J:98:PHE:CE1	2.42	0.55
1:G:333:ALA:HB2	1:G:344:VAL:HG11	1.88	0.55
1:C:93:VAL:HG23	1:C:100:PHE:HA	1.88	0.55
1:A:216:HIS:HD2	1:A:218:ARG:HB2	1.72	0.55
2:I:82:VAL:HG23	2:I:98:PHE:CE1	2.42	0.55
2:I:82:VAL:HG23	2:I:98:PHE:HE1	1.72	0.55
1:C:245:VAL:HG22	1:C:256:ARG:HB2	1.87	0.55
1:A:93:VAL:HG23	1:A:100:PHE:HA	1.88	0.55
1:A:245:VAL:HG22	1:A:256:ARG:HB2	1.89	0.55
2:I:47:TYR:HA	1:C:190:ARG:NH2	2.22	0.55
1:C:23:LYS:HA	1:C:58:ALA:HB1	1.87	0.55
1:G:337:LEU:HD22	1:G:337:LEU:H	1.72	0.54
1:C:433:ARG:HH21	1:C:434:ASN:ND2	2.02	0.54
2:K:114:GLN:HB3	2:K:122:ARG:HB3	1.89	0.54
1:A:274:VAL:HG12	1:A:278:CYS:HB2	1.88	0.54
1:E:304:THR:HG22	1:E:311:VAL:O	2.08	0.54
1:A:136:ALA:O	1:A:309:HIS:HA	2.07	0.54
2:J:82:VAL:HG23	2:J:98:PHE:HE1	1.71	0.54
1:A:304:THR:HG22	1:A:311:VAL:O	2.08	0.54
2:K:82:VAL:HG23	2:K:98:PHE:HE1	1.73	0.54
1:G:216:HIS:HD2	1:G:218:ARG:HB2	1.72	0.54
1:C:179:PRO:HG2	1:C:191:VAL:HG21	1.90	0.54



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:216:HIS:HD2	1:E:218:ARG:HB2	1.72	0.54
1:C:337:LEU:HD22	1:C:337:LEU:H	1.73	0.53
1:G:433:ARG:HH21	1:G:434:ASN:ND2	2.01	0.53
2:L:82:VAL:HG23	2:L:98:PHE:HE1	1.73	0.53
2:K:82:VAL:HG23	2:K:98:PHE:CE1	2.43	0.53
1:G:304:THR:HG22	1:G:311:VAL:O	2.08	0.53
1:E:274:VAL:HG12	1:E:278:CYS:HB2	1.89	0.53
1:E:337:LEU:HD22	1:E:337:LEU:H	1.72	0.53
1:G:93:VAL:HG23	1:G:100:PHE:HA	1.89	0.53
2:J:116:GLU:HB3	2:J:117:PRO:HD2	1.91	0.53
1:G:318:LYS:HG2	1:G:350:VAL:HG13	1.90	0.53
1:E:294:HIS:HA	1:E:327:HIS:HB2	1.91	0.53
1:G:420:THR:HG23	2:L:10:PHE:CE2	2.38	0.53
2:K:47:TYR:HA	1:G:190:ARG:NH2	2.23	0.53
1:E:93:VAL:HG23	1:E:100:PHE:HA	1.89	0.53
2:L:114:GLN:HB3	2:L:122:ARG:HB3	1.91	0.53
1:C:274:VAL:HG12	1:C:278:CYS:HB2	1.89	0.53
2:K:1:MET:SD	2:K:107:PRO:HD2	2.48	0.53
2:L:11:LEU:HB3	2:L:12:PRO:HD2	1.91	0.53
1:C:304:THR:HG22	1:C:311:VAL:O	2.09	0.52
1:A:190:ARG:NH2	2:L:47:TYR:HA	2.24	0.52
2:L:15:THR:H	2:L:18:GLN:HE21	1.56	0.52
1:C:216:HIS:HD2	1:C:218:ARG:HB2	1.74	0.52
1:E:333:ALA:HB2	1:E:344:VAL:HG11	1.90	0.52
2:I:1:MET:SD	2:I:107:PRO:HD2	2.49	0.52
2:I:114:GLN:HB3	2:I:122:ARG:HB3	1.92	0.52
2:J:114:GLN:HB3	2:J:122:ARG:HB3	1.92	0.52
2:L:82:VAL:HG23	2:L:98:PHE:CE1	2.43	0.52
1:A:318:LYS:HG2	1:A:350:VAL:HG13	1.92	0.52
1:C:83:TYR:HA	1:C:110:LEU:HD21	1.92	0.52
1:G:179:PRO:HG2	1:G:191:VAL:HG21	1.91	0.52
1:G:381:SER:HB3	3:G:507:PO4:O3	2.10	0.52
1:C:294:HIS:HA	1:C:327:HIS:HB2	1.92	0.52
2:K:104:ALA:HB1	2:K:107:PRO:HG3	1.92	0.52
1:G:294:HIS:HA	1:G:327:HIS:HB2	1.92	0.51
1:A:179:PRO:HG2	1:A:191:VAL:HG21	1.91	0.51
2:K:11:LEU:HB3	2:K:12:PRO:HD2	1.93	0.51
1:A:294:HIS:HA	1:A:327:HIS:HB2	1.93	0.51
2:J:1:MET:SD	2:J:107:PRO:HD2	2.50	0.51
2:J:11:LEU:HB3	2:J:12:PRO:HD2	1.92	0.51
2:J:104:ALA:HB1	2:J:107:PRO:HG3	1.93	0.51



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:262:SER:HA	2:K:117:PRO:HB3	1.92	0.51
1:E:178:LYS:HB3	1:E:409:ILE:HG21	1.93	0.51
1:G:64:SER:HB2	1:G:122:SER:O	2.11	0.51
2:J:47:TYR:OH	1:E:189:GLY:HA3	2.10	0.51
2:L:104:ALA:HB1	2:L:107:PRO:HG3	1.92	0.51
2:K:17:GLU:O	2:K:21:LYS:HG3	2.11	0.50
1:C:295:LEU:HB2	1:C:325:VAL:CG1	2.42	0.50
1:E:295:LEU:HB2	1:E:325:VAL:CG1	2.41	0.50
2:I:11:LEU:HB3	2:I:12:PRO:HD2	1.94	0.50
2:I:47:TYR:OH	1:C:189:GLY:HA3	2.12	0.50
2:I:104:ALA:HB1	2:I:107:PRO:HG3	1.94	0.50
1:E:318:LYS:HG2	1:E:350:VAL:HG13	1.92	0.50
1:E:64:SER:HB2	1:E:122:SER:O	2.11	0.50
2:L:1:MET:SD	2:L:107:PRO:HD2	2.51	0.50
2:L:116:GLU:HB3	2:L:117:PRO:HD2	1.94	0.50
2:I:116:GLU:HB3	2:I:117:PRO:HD2	1.93	0.49
1:A:183:LEU:HG	2:L:90:THR:HG21	1.95	0.49
2:K:47:TYR:OH	1:G:189:GLY:HA3	2.12	0.49
1:E:427:GLU:HG3	2:K:10:PHE:HB2	1.94	0.49
1:C:318:LYS:HG2	1:C:350:VAL:HG13	1.93	0.49
1:G:178:LYS:HB3	1:G:409:ILE:HG21	1.94	0.49
1:G:333:ALA:O	1:G:334:VAL:HG12	2.13	0.49
2:L:4:THR:O	2:L:4:THR:HG22	2.13	0.49
2:K:4:THR:HG22	2:K:4:THR:O	2.12	0.49
2:L:17:GLU:O	2:L:21:LYS:HG3	2.13	0.49
1:A:333:ALA:O	1:A:334:VAL:HG12	2.13	0.49
1:G:271:ASP:O	1:G:274:VAL:HG23	2.13	0.49
1:G:295:LEU:HB2	1:G:325:VAL:CG1	2.43	0.49
1:A:29:ASP:HB3	1:A:32:TYR:HB2	1.95	0.48
1:G:27:TYR:CZ	1:G:67:ALA:HB2	2.48	0.48
1:A:429:MET:HE2	1:A:439:ILE:HG23	1.94	0.48
1:A:178:LYS:HB3	1:A:409:ILE:HG21	1.94	0.48
2:K:116:GLU:HB3	2:K:117:PRO:HD2	1.94	0.48
1:C:271:ASP:O	1:C:274:VAL:HG23	2.13	0.48
1:E:45:ILE:HG22	1:E:47:PRO:HD3	1.95	0.48
2:I:4:THR:O	2:I:4:THR:HG22	2.14	0.48
1:C:89:ARG:HB2	1:C:103:TYR:HB2	1.96	0.48
2:J:112:VAL:O	2:J:123:TYR:HA	2.12	0.48
1:G:40:LEU:O	1:G:141:MET:HA	2.12	0.48
1:G:89:ARG:HB2	1:G:103:TYR:HB2	1.96	0.48
1:G:120:THR:HG22	1:G:319:TRP:CH2	2.48	0.48



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:64:SER:HB2	1:A:122:SER:O	2.13	0.48
1:A:271:ASP:O	1:A:274:VAL:HG23	2.13	0.48
1:C:429:MET:CE	1:C:439:ILE:HG23	2.44	0.48
1:E:40:LEU:O	1:E:141:MET:HA	2.14	0.48
2:I:112:VAL:O	2:I:123:TYR:HA	2.13	0.48
1:C:64:SER:HB2	1:C:122:SER:O	2.13	0.48
1:E:333:ALA:O	1:E:334:VAL:HG12	2.13	0.48
2:I:117:PRO:HB3	1:G:262:SER:HA	1.95	0.48
1:C:27:TYR:CZ	1:C:67:ALA:HB2	2.49	0.48
1:C:178:LYS:HB3	1:C:409:ILE:HG21	1.96	0.48
1:E:295:LEU:HB2	1:E:325:VAL:HG11	1.96	0.48
1:C:245:VAL:HG13	1:C:253:MET:HG3	1.96	0.47
1:A:83:TYR:HA	1:A:110:LEU:HD21	1.95	0.47
2:I:17:GLU:O	2:I:21:LYS:HG3	2.14	0.47
2:J:4:THR:HG22	2:J:4:THR:O	2.14	0.47
2:J:17:GLU:O	2:J:21:LYS:HG3	2.14	0.47
1:E:83:TYR:HA	1:E:110:LEU:HD21	1.95	0.47
1:G:244:ASN:ND2	1:G:246:THR:H	2.12	0.47
1:A:124:ILE:O	1:A:127:VAL:HG22	2.14	0.47
1:C:144:PRO:HG2	1:C:147:TYR:HB2	1.97	0.47
1:C:295:LEU:HB2	1:C:325:VAL:HG11	1.95	0.47
1:E:262:SER:HA	2:L:117:PRO:HB3	1.96	0.47
1:C:124:ILE:O	1:C:127:VAL:HG22	2.14	0.47
2:L:112:VAL:O	2:L:123:TYR:HA	2.14	0.47
1:A:27:TYR:CZ	1:A:67:ALA:HB2	2.49	0.47
1:A:89:ARG:HB2	1:A:103:TYR:HB2	1.96	0.47
1:C:29:ASP:HB3	1:C:32:TYR:HB2	1.97	0.47
1:E:27:TYR:CZ	1:E:67:ALA:HB2	2.50	0.47
1:A:120:THR:HG22	1:A:319:TRP:CZ3	2.50	0.47
1:A:295:LEU:HB2	1:A:325:VAL:CG1	2.44	0.47
1:C:120:THR:HG22	1:C:319:TRP:CH2	2.49	0.47
1:E:89:ARG:HB2	1:E:103:TYR:HB2	1.97	0.47
1:E:433:ARG:HG3	1:E:439:ILE:CD1	2.45	0.47
1:C:333:ALA:O	1:C:334:VAL:HG12	2.14	0.47
2:J:46:THR:HG21	1:E:186:ARG:HG3	1.96	0.47
1:E:124:ILE:O	1:E:127:VAL:HG22	2.14	0.47
1:E:144:PRO:HG2	1:E:147:TYR:HB2	1.96	0.47
1:G:120:THR:HG22	1:G:319:TRP:CZ3	2.50	0.47
2:I:65:LEU:HA	2:I:68:ILE:HD12	1.97	0.47
1:C:171:PRO:HA	1:C:398:ASP:O	2.15	0.47
1:A:144:PRO:HG2	1:A:147:TYR:HB2	1.96	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:I:113:ARG:HB3	2:I:121:LEU:HD22	1.96	0.46
1:C:244:ASN:ND2	1:C:246:THR:H	2.13	0.46
1:E:120:THR:HG22	1:E:319:TRP:CH2	2.50	0.46
1:A:120:THR:HG22	1:A:319:TRP:CH2	2.51	0.46
1:C:390:HIS:CD2	1:C:390:HIS:H	2.34	0.46
1:C:450:ALA:HA	1:C:453:TRP:NE1	2.31	0.46
1:E:271:ASP:O	1:E:274:VAL:HG23	2.15	0.46
1:A:431:LEU:HD12	2:I:22:GLN:OE1	2.15	0.46
1:E:120:THR:HG22	1:E:319:TRP:CZ3	2.50	0.46
1:E:429:MET:CE	1:E:439:ILE:HG23	2.46	0.46
1:C:433:ARG:HG3	1:C:439:ILE:CD1	2.45	0.46
1:G:124:ILE:O	1:G:127:VAL:HG22	2.15	0.46
1:A:80:CYS:O	1:A:82:MET:N	2.49	0.46
1:E:415:ILE:HD12	1:E:415:ILE:H	1.81	0.46
1:A:245:VAL:HG13	1:A:253:MET:HG3	1.97	0.46
1:A:433:ARG:HG3	1:A:439:ILE:CD1	2.46	0.46
1:E:245:VAL:HG13	1:E:253:MET:HG3	1.98	0.46
1:G:390:HIS:CD2	1:G:390:HIS:H	2.33	0.46
1:A:262:SER:HA	2:J:117:PRO:HB3	1.98	0.46
1:E:29:ASP:HB3	1:E:32:TYR:HB2	1.97	0.46
2:K:112:VAL:O	2:K:123:TYR:HA	2.16	0.46
1:G:450:ALA:HA	1:G:453:TRP:NE1	2.31	0.46
1:A:45:ILE:HG22	1:A:47:PRO:HD3	1.97	0.46
1:G:429:MET:CE	1:G:439:ILE:HG23	2.46	0.46
1:G:29:ASP:HB3	1:G:32:TYR:HB2	1.97	0.45
1:A:244:ASN:ND2	1:A:246:THR:H	2.15	0.45
2:K:65:LEU:HA	2:K:68:ILE:HD12	1.99	0.45
1:A:171:PRO:HA	1:A:398:ASP:O	2.15	0.45
1:G:42:LEU:HD13	1:G:139:GLU:HB2	1.98	0.45
1:G:69:TRP:HD1	1:G:69:TRP:H	1.64	0.45
1:G:285:TRP:CZ3	1:G:291:MET:HG3	2.51	0.45
1:E:450:ALA:HA	1:E:453:TRP:NE1	2.31	0.45
1:E:171:PRO:HA	1:E:398:ASP:O	2.17	0.45
1:E:244:ASN:ND2	1:E:246:THR:H	2.15	0.45
1:E:429:MET:HE2	1:E:439:ILE:HG23	1.98	0.45
2:K:46:THR:HG21	1:G:186:ARG:HG3	1.97	0.45
1:A:390:HIS:H	1:A:390:HIS:CD2	2.35	0.45
1:A:450:ALA:HA	1:A:453:TRP:NE1	2.31	0.45
1:E:455:GLY:O	1:E:458:ARG:HB3	2.16	0.45
1:G:171:PRO:HA	1:G:398:ASP:O	2.16	0.45
2:I:109:PHE:HD1	2:I:109:PHE:H	1.64	0.45



	, and pagetti	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:120:THR:HG22	1:C:319:TRP:CZ3	2.51	0.45
1:C:429:MET:HE2	1:C:439:ILE:HG23	1.98	0.45
1:E:69:TRP:HD1	1:E:69:TRP:H	1.65	0.45
1:E:135:ALA:HB1	1:E:308:ASN:O	2.17	0.45
1:A:40:LEU:O	1:A:141:MET:HA	2.16	0.45
1:A:415:ILE:HD12	1:A:415:ILE:H	1.81	0.45
1:C:40:LEU:O	1:C:141:MET:HA	2.16	0.45
2:L:65:LEU:HA	2:L:68:ILE:HD12	1.97	0.45
1:C:80:CYS:O	1:C:82:MET:N	2.50	0.45
1:E:390:HIS:CD2	1:E:390:HIS:H	2.35	0.45
1:G:144:PRO:HG2	1:G:147:TYR:HB2	1.98	0.45
1:C:45:ILE:HG22	1:C:47:PRO:HD3	1.98	0.45
1:A:429:MET:CE	1:A:439:ILE:HG23	2.46	0.44
1:C:455:GLY:O	1:C:458:ARG:HB3	2.17	0.44
1:E:385:HIS:HE1	1:E:465:GLY:O	2.00	0.44
1:G:83:TYR:HA	1:G:110:LEU:HD21	1.97	0.44
1:G:135:ALA:HB1	1:G:308:ASN:O	2.17	0.44
1:G:429:MET:HE2	1:G:439:ILE:HG23	1.98	0.44
2:J:109:PHE:HD1	2:J:109:PHE:H	1.66	0.44
1:E:295:LEU:CB	1:E:325:VAL:HG11	2.47	0.44
1:G:295:LEU:HB2	1:G:325:VAL:HG11	1.98	0.44
1:A:295:LEU:HB2	1:A:325:VAL:HG11	1.99	0.44
2:J:113:ARG:HB3	2:J:121:LEU:HD22	1.98	0.44
1:E:80:CYS:O	1:E:82:MET:N	2.50	0.44
2:L:109:PHE:H	2:L:109:PHE:HD1	1.65	0.44
1:C:173:LEU:HD13	1:C:200:LEU:HD23	1.99	0.44
2:J:37:TYR:HA	2:J:79:TYR:O	2.18	0.44
1:E:336:LYS:HG3	1:E:383:GLY:N	2.33	0.44
1:G:80:CYS:O	1:G:82:MET:N	2.51	0.44
1:G:245:VAL:HG13	1:G:253:MET:HG3	1.99	0.44
1:A:455:GLY:O	1:A:458:ARG:HB3	2.17	0.44
1:C:415:ILE:HD12	1:C:415:ILE:H	1.83	0.44
1:C:431:LEU:HD12	2:J:22:GLN:OE1	2.18	0.44
1:E:303:TYR:CD1	1:E:304:THR:HG23	2.53	0.44
1:G:45:ILE:HG22	1:G:47:PRO:HD3	2.00	0.44
1:G:385:HIS:HE1	1:G:465:GLY:O	1.99	0.44
1:C:427:GLU:HG3	2:J:10:PHE:HB2	2.00	0.44
2:J:65:LEU:HA	2:J:68:ILE:HD12	1.98	0.44
2:J:104:ALA:O	2:J:105:ASP:C	2.55	0.44
1:C:340:ASP:O	1:C:344:VAL:HG23	2.18	0.44
1:G:427:GLU:HG3	2:L:10:PHE:HB2	2.00	0.44



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:G:455:GLY:O	1:G:458:ARG:HB3	2.17	0.44
1:E:439:ILE:H	1:E:439:ILE:HG13	1.56	0.44
1:G:340:ASP:O	1:G:344:VAL:HG23	2.18	0.44
1:A:340:ASP:O	1:A:344:VAL:HG23	2.18	0.43
1:C:295:LEU:CB	1:C:325:VAL:HG11	2.48	0.43
1:C:385:HIS:HE1	1:C:465:GLY:O	2.01	0.43
1:A:283:SER:OG	1:A:324:GLY:HA3	2.18	0.43
1:A:385:HIS:HE1	1:A:465:GLY:O	2.00	0.43
1:G:336:LYS:HG3	1:G:383:GLY:N	2.33	0.43
1:C:180:LYS:HG3	1:C:206:ASP:HB3	2.00	0.43
2:K:37:TYR:HA	2:K:79:TYR:O	2.19	0.43
2:K:104:ALA:O	2:K:105:ASP:C	2.56	0.43
1:G:433:ARG:HG3	1:G:439:ILE:CD1	2.47	0.43
1:C:283:SER:OG	1:C:324:GLY:HA3	2.18	0.43
1:C:336:LYS:HG3	1:C:383:GLY:N	2.33	0.43
2:I:37:TYR:HA	2:I:79:TYR:O	2.18	0.43
1:C:135:ALA:HB1	1:C:308:ASN:O	2.19	0.43
2:K:109:PHE:HD1	2:K:109:PHE:H	1.64	0.43
1:G:415:ILE:HD12	1:G:415:ILE:H	1.84	0.43
1:A:69:TRP:H	1:A:69:TRP:HD1	1.66	0.43
2:I:45:ASN:ND2	2:J:113:ARG:HH22	2.16	0.43
1:E:42:LEU:HD13	1:E:139:GLU:HB2	1.99	0.43
2:L:37:TYR:HA	2:L:79:TYR:O	2.18	0.43
2:I:113:ARG:HH22	2:L:45:ASN:ND2	2.17	0.43
1:G:295:LEU:CB	1:G:325:VAL:HG11	2.49	0.43
1:A:135:ALA:HB1	1:A:308:ASN:O	2.19	0.43
2:K:113:ARG:HB3	2:K:121:LEU:HD22	2.01	0.43
1:A:144:PRO:HG2	1:A:147:TYR:CB	2.49	0.43
2:K:68:ILE:HD13	2:K:98:PHE:CE1	2.53	0.43
2:K:90:THR:HG21	1:G:183:LEU:HG	2.01	0.43
2:I:104:ALA:O	2:I:105:ASP:C	2.56	0.42
1:C:69:TRP:HD1	1:C:69:TRP:H	1.65	0.42
1:E:56:ALA:O	1:E:60:VAL:HG23	2.19	0.42
1:E:144:PRO:HG2	1:E:147:TYR:CB	2.48	0.42
1:E:245:VAL:HG22	1:E:256:ARG:CB	2.49	0.42
1:E:283:SER:OG	1:E:324:GLY:HA3	2.18	0.42
2:L:104:ALA:O	2:L:105:ASP:C	2.56	0.42
2:I:68:ILE:HD13	2:I:98:PHE:CE1	2.54	0.42
1:C:56:ALA:O	1:C:60:VAL:HG23	2.20	0.42
2:K:38:THR:HG22	2:K:39:ASP:N	2.35	0.42
1:G:173:LEU:HD13	1:G:200:LEU:HD23	2.01	0.42



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:L:77:ASN:HD21	2:L:102:ARG:HE	1.67	0.42
1:A:336:LYS:HG3	1:A:383:GLY:N	2.33	0.42
1:C:80:CYS:HB2	1:C:84:ARG:HG3	2.02	0.42
1:E:173:LEU:HD13	1:E:200:LEU:HD23	2.02	0.42
1:E:180:LYS:HG3	1:E:206:ASP:HB3	2.02	0.42
1:A:209:ILE:O	1:A:209:ILE:HG13	2.18	0.42
1:G:180:LYS:HG3	1:G:206:ASP:HB3	2.01	0.42
2:L:68:ILE:HD13	2:L:98:PHE:CE1	2.54	0.42
2:J:68:ILE:HD13	2:J:98:PHE:CE1	2.55	0.42
1:E:340:ASP:O	1:E:344:VAL:HG23	2.20	0.42
1:A:303:TYR:CD1	1:A:304:THR:HG23	2.54	0.42
1:E:285:TRP:CZ3	1:E:291:MET:HG3	2.54	0.42
1:C:161:GLU:HG3	1:C:292:ILE:HD13	2.02	0.42
2:J:77:ASN:HD21	2:J:102:ARG:HE	1.68	0.42
2:J:104:ALA:O	2:J:106:GLU:N	2.53	0.42
1:G:56:ALA:O	1:G:60:VAL:HG23	2.20	0.42
1:G:242:TYR:CD1	1:G:267:ILE:HD13	2.55	0.42
2:J:38:THR:HG22	2:J:39:ASP:N	2.35	0.41
2:K:104:ALA:O	2:K:106:GLU:N	2.54	0.41
2:L:104:ALA:O	2:L:106:GLU:N	2.53	0.41
1:A:80:CYS:HB2	1:A:84:ARG:HG3	2.03	0.41
2:I:63:GLY:O	2:I:66:MET:HB3	2.21	0.41
2:I:119:ARG:HH21	2:L:44:ARG:HG3	1.85	0.41
1:C:209:ILE:HG13	1:C:209:ILE:O	2.21	0.41
1:E:78:THR:C	1:E:80:CYS:H	2.24	0.41
1:C:78:THR:C	1:C:80:CYS:H	2.24	0.41
1:C:439:ILE:H	1:C:439:ILE:HG13	1.58	0.41
1:G:144:PRO:HG2	1:G:147:TYR:CB	2.50	0.41
1:G:303:TYR:CD1	1:G:304:THR:HG23	2.55	0.41
2:L:108:GLY:O	2:L:128:TYR:HE1	2.03	0.41
2:L:113:ARG:HB3	2:L:121:LEU:HD22	2.01	0.41
1:C:154:PRO:HA	1:C:324:GLY:HA2	2.02	0.41
1:C:155:SER:HA	1:C:287:ARG:HD3	2.03	0.41
1:A:320:LEU:HD22	1:A:325:VAL:HG21	2.02	0.41
1:A:439:ILE:H	1:A:439:ILE:HG13	1.57	0.41
1:C:285:TRP:CZ3	1:C:291:MET:HG3	2.54	0.41
1:C:303:TYR:CD1	1:C:304:THR:HG23	2.55	0.41
1:A:42:LEU:HD13	1:A:139:GLU:HB2	2.02	0.41
1:A:173:LEU:HD13	1:A:200:LEU:HD23	2.03	0.41
1:C:144:PRO:HG2	1:C:147:TYR:CB	2.50	0.41
1:C:314:ARG:HB3	1:C:347:TYR:CE1	2.56	0.41



Atom 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:E:242:TYR:CD1	1:E:267:ILE:HD13	2.56	0.41
2:K:77:ASN:HD21	2:K:102:ARG:HE	1.68	0.41
2:L:33:VAL:HG13	2:L:82:VAL:HG13	2.03	0.41
2:L:38:THR:HG22	2:L:39:ASP:N	2.36	0.41
1:A:56:ALA:O	1:A:60:VAL:HG23	2.20	0.41
1:A:78:THR:C	1:A:80:CYS:H	2.24	0.41
1:A:154:PRO:HA	1:A:324:GLY:HA2	2.03	0.41
1:G:78:THR:C	1:G:80:CYS:H	2.24	0.41
2:L:19:ILE:O	2:L:23:LEU:HG	2.21	0.41
1:A:285:TRP:CZ3	1:A:291:MET:HG3	2.56	0.41
2:J:82:VAL:CG2	2:J:98:PHE:CE1	3.04	0.41
1:E:39:LEU:HG	1:E:111:PHE:CE1	2.56	0.41
1:G:431:LEU:HD12	2:L:22:GLN:OE1	2.21	0.41
1:A:180:LYS:HG3	1:A:206:ASP:HB3	2.02	0.40
2:I:104:ALA:O	2:I:106:GLU:N	2.54	0.40
1:C:245:VAL:HG13	1:C:245:VAL:O	2.21	0.40
1:A:254:TYR:OH	1:A:281:SER:HB3	2.20	0.40
1:C:179:PRO:CB	1:C:183:LEU:HD22	2.52	0.40
1:E:80:CYS:HB2	1:E:84:ARG:HG3	2.03	0.40
1:E:209:ILE:O	1:E:209:ILE:HG13	2.21	0.40
2:K:108:GLY:O	2:K:128:TYR:HE1	2.04	0.40
2:K:82:VAL:CG2	2:K:98:PHE:CE1	3.04	0.40
2:K:119:ARG:HD2	2:K:119:ARG:HA	1.85	0.40
1:G:155:SER:HA	1:G:287:ARG:HD3	2.04	0.40
2:L:42:HIS:HB3	2:L:45:ASN:HB2	2.04	0.40
1:A:39:LEU:HG	1:A:111:PHE:CE1	2.56	0.40
1:A:178:LYS:HA	1:A:178:LYS:HD2	1.99	0.40
1:A:274:VAL:HG12	1:A:278:CYS:SG	2.61	0.40
1:A:314:ARG:HB3	1:A:347:TYR:CE1	2.56	0.40
2:I:119:ARG:HA	2:I:119:ARG:HD2	1.82	0.40
2:J:108:GLY:O	2:J:128:TYR:HE1	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Pe	erce	entil	$\mathbf{es}$
1	А	443/485~(91%)	390~(88%)	41 (9%)	12 (3%)		5	12	
1	С	443/485~(91%)	389~(88%)	43 (10%)	11 (2%)		5	14	
1	Е	443/485~(91%)	390 (88%)	42 (10%)	11 (2%)		5	14	
1	G	443/485~(91%)	389~(88%)	44 (10%)	10 (2%)		6	16	
2	Ι	127/139~(91%)	104 (82%)	18 (14%)	5 (4%)		3	6	
2	J	127/139~(91%)	104 (82%)	18 (14%)	5 (4%)		3	6	
2	K	127/139~(91%)	104 (82%)	19 (15%)	4 (3%)		4	9	
2	L	127/139~(91%)	104 (82%)	18 (14%)	5 (4%)		3	6	
All	All	2280/2496~(91%)	1974 (87%)	243 (11%)	63 (3%)		5	11	

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

All (63) Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	207	GLU
2	Ι	103	PRO
2	Ι	105	ASP
1	С	207	GLU
2	J	103	PRO
2	J	105	ASP
1	Е	207	GLU
2	Κ	103	PRO
2	Κ	105	ASP
1	G	207	GLU
2	L	103	PRO
2	L	105	ASP
1	А	81	ASP
1	А	214	PHE
1	А	308	ASN
2	Ι	56	PHE
1	С	81	ASP
1	С	214	PHE
1	С	308	ASN
2	J	56	PHE
1	Е	81	ASP
1	Е	214	PHE
1	Е	308	ASN
2	K	56	PHE



Mal	Chain	<b>B</b> oo	
1	Cliain	01	лер
1	G	014	ASP
1 1	G	214	PHE
1	G	308	ASN
2		56	PHE
1	A	25	MET
1	A	80	CYS
1	A	211	SER
1	C	25	MET
1	C	80	CYS
1	C	211	SER
1	E	25	MET
1	E	80	CYS
1	Е	211	SER
1	E	333	ALA
1	G	25	MET
1	G	80	CYS
1	G	211	SER
1	А	333	ALA
1	А	440	LEU
2	Ι	104	ALA
1	С	333	ALA
1	С	440	LEU
2	J	104	ALA
1	Е	440	LEU
2	Κ	104	ALA
1	G	333	ALA
1	G	440	LEU
2	L	104	ALA
2	Ι	47	TYR
1	А	66	THR
1	А	371	ALA
1	С	66	THR
2	J	47	TYR
1	Е	66	THR
2	L	47	TYR
1	А	334	VAL
1	С	334	VAL
1	Е	334	VAL
1	G	334	VAL



#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	358/391~(92%)	343~(96%)	15~(4%)	30	58
1	С	358/391~(92%)	343~(96%)	15 (4%)	30	58
1	Ε	358/391~(92%)	343~(96%)	15~(4%)	30	58
1	G	358/391~(92%)	343~(96%)	15 (4%)	30	58
2	Ι	115/122~(94%)	105~(91%)	10 (9%)	10	23
2	J	115/122~(94%)	105~(91%)	10 (9%)	10	23
2	Κ	115/122~(94%)	105~(91%)	10 (9%)	10	23
2	L	115/122~(94%)	$105 \ (91\%)$	10 (9%)	10	23
All	All	1892/2052~(92%)	1792 (95%)	100 (5%)	22	48

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	25	MET
1	А	42	LEU
1	А	68	THR
1	А	75	ASP
1	А	80	CYS
1	А	119	LEU
1	А	173	LEU
1	А	183	LEU
1	А	244	ASN
1	А	245	VAL
1	А	271	ASP
1	А	272	LEU
1	А	287	ARG
1	А	334	VAL
1	А	377	MET
2	Ι	10	PHE
2	Ι	44	ARG
2	Ι	49	GLU
2	Ι	59	ARG



Mol	Chain	Res	Type
2	Ι	70	ASN
2	Ι	96	MET
2	Ι	99	ILE
2	Ι	103	PRO
2	Ι	110	ARG
2	Ι	122	ARG
1	С	25	MET
1	С	42	LEU
1	С	68	THR
1	С	75	ASP
1	С	80	CYS
1	С	119	LEU
1	С	173	LEU
1	С	183	LEU
1	С	244	ASN
1	С	245	VAL
1	С	271	ASP
1	С	272	LEU
1	С	287	ARG
1	С	334	VAL
1	С	377	MET
2	J	10	PHE
2	J	44	ARG
2	J	49	GLU
2	J	59	ARG
2	J	70	ASN
2	J	96	MET
2	J	99	ILE
$2^{-}$	J	$10\overline{3}$	PRO
2	J	110	ARG
2	J	122	ARG
1	E	25	MET
1	Е	42	LEU
1	E	68	THR
1	E	75	ASP
1	E	80	CYS
1	Е	119	LEU
1	Е	173	LEU
1	E	183	LEU
1	Е	244	ASN
1	E	245	VAL
1	Ε	271	ASP



Mol	Chain	Res	Type
1	Е	272	LEU
1	Е	287	ARG
1	Е	334	VAL
1	Е	377	MET
2	К	10	PHE
2	К	44	ARG
2	K	49	GLU
2	Κ	59	ARG
2	K	70	ASN
2	Κ	96	MET
2	Κ	99	ILE
2	Κ	103	PRO
2	Κ	110	ARG
2	K	122	ARG
1	G	25	MET
1	G	42	LEU
1	G	68	THR
1	G	75	ASP
1	G	80	CYS
1	G	119	LEU
1	G	173	LEU
1	G	183	LEU
1	G	244	ASN
1	G	245	VAL
1	G	271	ASP
1	G	272	LEU
1	G	287	ARG
1	G	334	VAL
1	G	377	MET
2	L	10	PHE
2	L	44	ARG
2	L	49	GLU
2	L	59	ARG
2	L	70	ASN
2	L	96	MET
2	L	99	ILE
2	L	103	PRO
2	L	110	ARG
2	L	122	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:



Mol	Chain	Res	Type
1	А	210	ASN
1	А	216	HIS
1	А	244	ASN
1	А	345	GLN
1	А	385	HIS
1	А	416	GLN
1	А	434	ASN
2	Ι	18	GLN
2	Ι	22	GLN
2	Ι	45	ASN
2	Ι	70	ASN
2	Ι	77	ASN
2	Ι	78	HIS
1	С	210	ASN
1	С	216	HIS
1	С	244	ASN
1	С	345	GLN
1	С	385	HIS
1	С	416	GLN
1	С	434	ASN
2	J	18	GLN
2	J	22	GLN
2	J	45	ASN
2	J	70	ASN
2	J	78	HIS
1	Е	210	ASN
1	Е	216	HIS
1	Е	244	ASN
1	Е	345	GLN
1	Е	385	HIS
1	Е	416	GLN
1	Е	434	ASN
2	K	18	GLN
2	K	22	GLN
2	K	45	ASN
2	K	70	ASN
2	K	78	HIS
1	G	210	ASN
1	G	216	HIS
1	G	244	ASN
1	G	345	GLN
1	G	385	HIS
1	G	416	GLN



Continued from previous page...

Mol	Chain	Res	Type
1	G	434	ASN
2	L	18	GLN
2	L	22	GLN
2	L	45	ASN
2	L	70	ASN
2	L	77	ASN
2	L	78	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)

8 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).

Mal	Jol Type Chain Res Link		Tiple	Bond lengths			Bond angles			
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	PO4	E	506	-	4,4,4	1.45	1 (25%)	6,6,6	1.02	0
3	PO4	С	504	-	4,4,4	1.65	1 (25%)	6,6,6	1.04	0
3	PO4	А	502	-	4,4,4	1.58	1 (25%)	6,6,6	1.07	0
3	PO4	С	503	-	4,4,4	1.73	1 (25%)	6,6,6	1.08	0
3	PO4	E	505	-	4,4,4	1.58	1 (25%)	6,6,6	1.11	0



Mal	Turne	Chain	Dec	Tink	B	ond leng	$\operatorname{gths}$	E	Bond ang	gles
	Type	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	PO4	G	507	-	4,4,4	1.77	1 (25%)	6,6,6	1.12	0
3	PO4	А	501	-	4,4,4	1.71	1 (25%)	6,6,6	1.10	0
3	PO4	G	508	-	4,4,4	1.56	1 (25%)	6,6,6	1.13	0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
3	А	501	PO4	P-O3	-3.17	1.45	1.54
3	С	503	PO4	P-O3	-3.17	1.45	1.54
3	G	507	PO4	P-O3	-3.13	1.45	1.54
3	А	502	PO4	P-O3	-2.93	1.45	1.54
3	С	504	PO4	P-O3	-2.92	1.45	1.54
3	Е	505	PO4	P-O3	-2.91	1.45	1.54
3	G	508	PO4	P-O3	-2.80	1.46	1.54
3	Е	506	PO4	P-O3	-2.61	1.46	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	507	PO4	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,  $95^{th}$  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 $>$	#RSR	RZ>	2	$OWAB(Å^2)$	Q<0.9
1	А	445/485~(91%)	0.20	38 (8%)	10	9	2, 29, 99, 100	0
1	С	445/485~(91%)	0.20	43 (9%)	7	6	2, 28, 98, 100	0
1	Ε	445/485~(91%)	0.38	49 (11%)	5	4	2, 31, 100, 100	0
1	G	445/485~(91%)	0.18	38~(8%)	10	9	2, 26, 98, 100	0
2	Ι	129/139~(92%)	0.46	14 (10%)	5	4	4, 35, 99, 100	0
2	J	129/139~(92%)	0.55	17 (13%)	3	2	2, 40, 100, 100	0
2	Κ	129/139~(92%)	0.59	14 (10%)	5	4	3, 41, 98, 100	0
2	L	129/139~(92%)	0.47	16 (12%)	4	3	2, 36, 100, 100	0
All	All	2296/2496~(91%)	0.30	229 (9%)	7	5	2, 31, 100, 100	0

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	72	VAL	12.4
1	G	72	VAL	11.9
1	Е	337	LEU	10.1
1	С	72	VAL	9.8
1	А	74	THR	9.7
1	А	68	THR	9.4
1	G	181	LEU	9.3
1	А	69	TRP	9.1
1	G	73	TRP	9.1
2	Κ	105	ASP	8.9
1	Е	66	THR	8.7
1	Е	181	LEU	8.6
1	С	337	LEU	8.4
1	G	337	LEU	7.9
1	Е	339	GLY	7.9
1	Ε	71	VAL	7.6



Mol	Chain	Res	Type	RSRZ
2	L	105	ASP	7.6
1	G	77	LEU	7.6
1	А	73	TRP	7.3
1	G	71	VAL	7.3
1	А	76	ARG	7.2
2	L	107	PRO	7.1
1	Е	338	GLU	7.0
1	С	68	THR	7.0
1	С	466	ASP	6.9
1	С	77	LEU	6.9
1	G	66	THR	6.8
1	Е	73	TRP	6.5
1	Е	82	MET	6.5
2	J	107	PRO	6.5
2	K	107	PRO	6.4
1	G	74	THR	6.4
1	А	181	LEU	6.2
2	Ι	107	PRO	5.8
1	Е	78	THR	5.8
1	Е	75	ASP	5.8
1	А	337	LEU	5.7
2	Ι	105	ASP	5.6
1	С	78	THR	5.5
1	С	76	ARG	5.5
1	С	181	LEU	5.5
1	G	68	THR	5.4
2	J	105	ASP	5.4
2	K	1	MET	5.2
1	А	66	THR	5.1
2	J	108	GLY	5.1
1	Е	340	ASP	5.1
1	G	69	TRP	5.0
1	G	67	ALA	5.0
1	А	338	GLU	4.9
1	G	334	VAL	4.9
1	Е	80	CYS	4.8
2	Κ	129	ALA	4.8
1	G	214	PHE	4.8
1	С	66	THR	4.8
1	С	82	MET	4.7
1	Е	465	GLY	4.7
1	С	73	TRP	4.7



Mol	Chain	Res	Type	RSRZ
1	Е	211	SER	4.7
1	G	75	ASP	4.6
1	С	69	TRP	4.6
1	С	79	ALA	4.6
1	А	339	GLY	4.6
1	А	72	VAL	4.6
1	Е	466	ASP	4.5
1	С	334	VAL	4.5
1	С	71	VAL	4.4
1	G	76	ARG	4.4
2	Κ	108	GLY	4.4
2	Κ	98	PHE	4.4
1	Е	77	LEU	4.4
1	Е	214	PHE	4.3
2	Ι	59	ARG	4.3
1	Е	334	VAL	4.3
1	С	75	ASP	4.3
2	Κ	58	LEU	4.2
1	А	70	THR	4.2
1	С	180	LYS	4.1
1	А	211	SER	4.1
1	А	466	ASP	4.1
2	L	98	PHE	4.1
2	J	89	HIS	4.0
1	Е	81	ASP	3.9
2	L	108	GLY	3.9
1	Е	83	TYR	3.9
1	А	467	ILE	3.9
1	А	75	ASP	3.8
1	С	182	GLY	3.8
1	С	445	GLU	3.8
1	С	338	GLU	3.7
2	Ι	101	ASN	3.7
2	Ι	57	ASP	3.7
2	Κ	102	ARG	3.7
1	Е	95	ASN	3.7
1	С	467	ILE	3.7
1	G	78	THR	3.6
1	А	334	VAL	3.6
2	J	1	MET	3.5
1	Е	65	SER	3.5
1	А	210	ASN	3.5



Mol	Chain	Res	Type	RSRZ
1	Е	50	GLY	3.5
2	Ι	129	ALA	3.5
2	Ι	98	PHE	3.4
2	J	56	PHE	3.4
2	K	56	PHE	3.4
1	С	74	THR	3.4
1	Е	74	THR	3.3
1	G	182	GLY	3.3
1	G	22	TYR	3.3
1	Е	69	TRP	3.3
1	С	83	TYR	3.3
1	С	465	GLY	3.3
1	Е	98	GLU	3.3
1	Е	22	TYR	3.3
1	G	213	PRO	3.3
2	J	101	ASN	3.2
1	Е	467	ILE	3.2
2	L	57	ASP	3.2
1	А	81	ASP	3.2
2	K	59	ARG	3.2
1	G	338	GLU	3.2
2	L	89	HIS	3.2
1	С	33	VAL	3.2
2	Ι	88	THR	3.2
2	J	58	LEU	3.2
1	А	464	TRP	3.2
1	А	98	GLU	3.2
1	Е	207	GLU	3.1
1	Е	70	THR	3.1
1	А	78	THR	3.1
2	J	103	PRO	3.1
2	J	102	ARG	3.1
1	G	467	ILE	3.1
1	Е	79	ALA	3.0
1	Е	180	LYS	3.0
1	A	67	ALA	3.0
1	C	207	GLU	3.0
1	G	466	ASP	3.0
1	Е	464	TRP	3.0
1	С	208	ASN	2.9
1	Е	182	GLY	2.9
1	Е	131	LYS	2.9



Mol	Chain	Res	Type	RSRZ
1	С	210	ASN	2.9
2	L	88	THR	2.9
1	С	211	SER	2.9
2	Ι	102	ARG	2.9
2	L	129	ALA	2.9
1	С	439	ILE	2.8
2	L	58	LEU	2.8
2	J	21	LYS	2.8
1	Е	342	LEU	2.8
1	С	65	SER	2.7
2	J	95	VAL	2.7
1	Е	341	PRO	2.7
1	С	84	ARG	2.7
2	L	59	ARG	2.7
1	С	98	GLU	2.6
2	Ι	108	GLY	2.6
2	K	103	PRO	2.6
1	С	22	TYR	2.6
1	А	458	ARG	2.6
1	А	65	SER	2.6
2	Κ	57	ASP	2.6
1	G	82	MET	2.6
1	А	31	ASP	2.5
1	G	210	ASN	2.5
1	Е	67	ALA	2.5
1	А	22	TYR	2.5
1	G	211	SER	2.5
1	А	333	ALA	2.5
1	С	64	SER	2.5
2	Ι	89	HIS	2.5
1	A	80	CYS	2.5
1	G	207	GLU	2.5
1	G	98	GLU	2.5
1	A	180	LYS	2.5
1	А	71	VAL	2.4
2	L	60	ASP	2.4
1	A	414	GLY	2.4
1	Е	33	VAL	2.4
1	С	80	CYS	2.4
2	Κ	95	VAL	2.4
1	G	83	TYR	2.4
2	L	102	ARG	2.4



Mol	Chain	Res	Type	RSRZ
1	G	206	ASP	2.4
1	А	49	ASP	2.3
1	Е	26	GLY	2.3
2	K	90	THR	2.3
2	J	106	GLU	2.3
1	Е	426	LEU	2.3
1	G	464	TRP	2.3
1	Е	278	CYS	2.3
1	G	180	LYS	2.3
2	J	88	THR	2.2
1	А	207	GLU	2.2
1	А	82	MET	2.2
2	J	90	THR	2.2
1	G	439	ILE	2.2
2	Ι	103	PRO	2.2
1	С	464	TRP	2.2
1	С	70	THR	2.2
1	А	214	PHE	2.2
1	G	131	LYS	2.2
1	С	336	LYS	2.2
1	С	214	PHE	2.2
2	J	44	ARG	2.1
1	Ε	357	GLN	2.1
1	Е	52	ASP	2.1
1	G	49	ASP	2.1
1	G	452	ARG	2.1
1	G	332	THR	2.1
2	L	90	THR	2.1
1	Ε	441	ASN	2.1
1	С	67	ALA	2.1
1	Е	28	TRP	2.1
1	E	210	ASN	2.1
2	Ι	87	SER	2.1
2	L	44	ARG	2.1
2	J	129	ALA	2.1
1	С	95	ASN	2.1
2	L	1	MET	2.1
1	С	456	PRO	2.0
2	L	95	VAL	2.0
2	Ι	119	ARG	2.0
1	G	70	THR	2.0
1	Е	336	LYS	2.0



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	А	209	ILE	2.0
1	G	336	LYS	2.0
1	А	332	THR	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,  $95^{th}$  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	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9
3	PO4	G	508	5/5	0.92	0.24	18,23,40,42	0
3	PO4	Е	506	5/5	0.94	0.33	18,23,40,42	0
3	PO4	G	507	5/5	0.94	0.18	18,23,40,42	0
3	PO4	С	504	5/5	0.94	0.25	18,23,40,42	0
3	PO4	А	501	5/5	0.95	0.22	18,23,40,42	0
3	PO4	С	503	5/5	0.95	0.22	18,23,40,42	0
3	PO4	А	502	5/5	0.96	0.25	18,23,40,42	0
3	PO4	Е	505	5/5	0.97	0.20	18,23,40,42	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

