



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:16 AM GMT

PDB ID : 3A58  
Title : Crystal structure of Sec3p - Rho1p complex from *Saccharomyces cerevisiae*  
Authors : Yamashita, M.; Sato, Y.; Yamagata, A.; Mimura, H.; Yoshikawa, A.; Fukai, S.  
Deposited on : 2009-08-03  
Resolution : 2.60 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



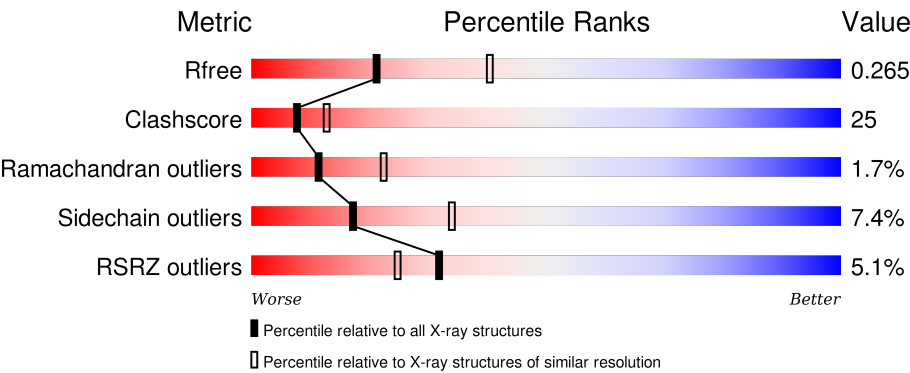
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	320	<div><div>2%</div><div>36%19%•42%</div></div>
1	C	320	<div><div>33%20%•44%</div></div>
1	E	320	<div><div>9%21%29%•48%</div></div>
2	B	188	<div><div>8%51%41%••5%</div></div>
2	D	188	<div><div>%65%24%6%5%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	188	<div><div><div>%</div><div><div></div></div><div>57%</div><div>34%</div><div>5% • •</div></div></div>



## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8792 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 Exocyst complex component SEC3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	Se	0	0	0
			1522	969	268	282	2	1			
1	C	180	Total	C	N	O	S	Se	0	0	0
			1485	944	262	276	2	1			
1	E	166	Total	C	N	O	S	Se	0	0	0
			1377	882	238	254	2	1			

- Molecule 2 is a protein called GTP-binding protein RHO1.

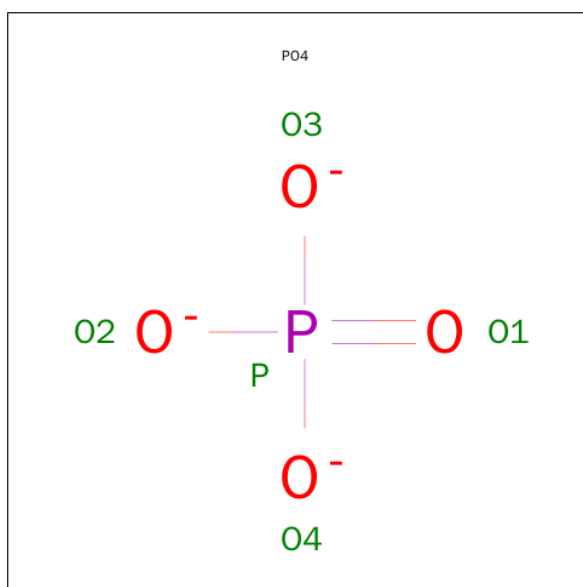
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1385	871	235	272	7			
2	D	178	Total	C	N	O	S	0	0	0
			1385	871	235	272	7			
2	F	181	Total	C	N	O	S	0	0	0
			1406	883	240	276	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	30	ASN	PHE	ENGINEERED	UNP P06780
D	30	ASN	PHE	ENGINEERED	UNP P06780
F	30	ASN	PHE	ENGINEERED	UNP P06780

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

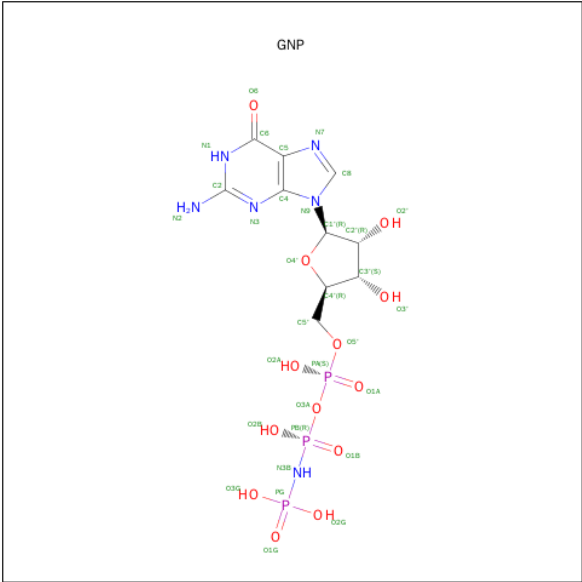




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	F	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total	O	0	0
			29	29		
6	B	7	Total	O	0	0
			7	7		
6	C	24	Total	O	0	0
			24	24		

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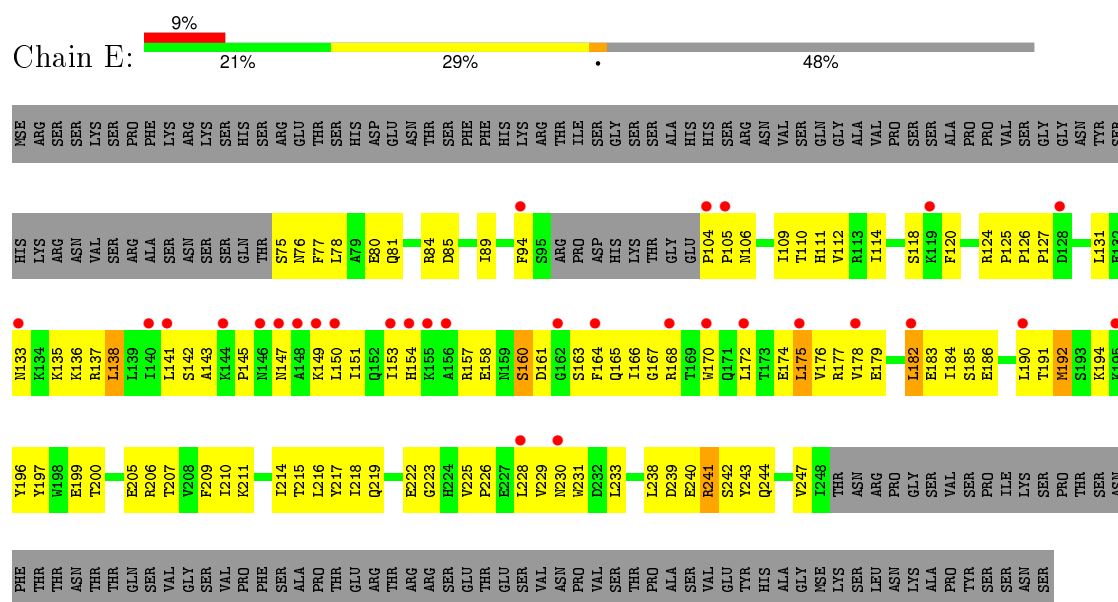
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	25	Total 25	O 25	0	0
6	E	6	Total 6	O 6	0	0
6	F	7	Total 7	O 7	0	0

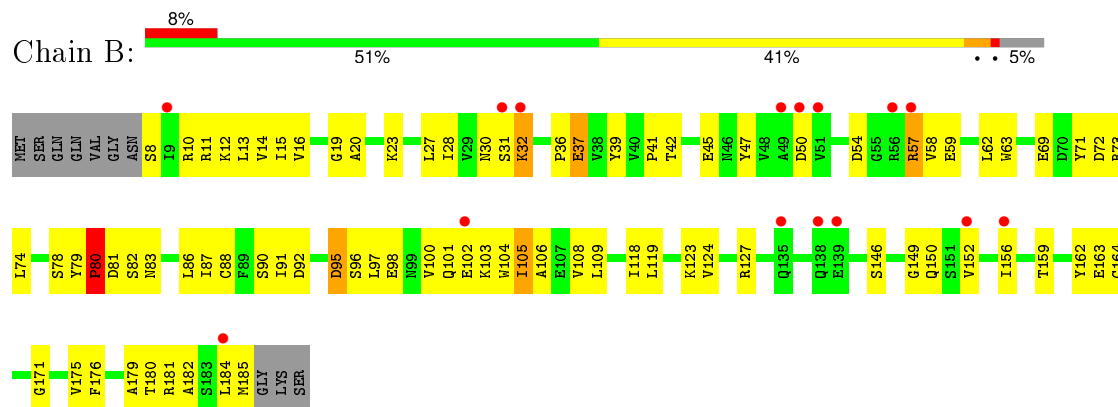




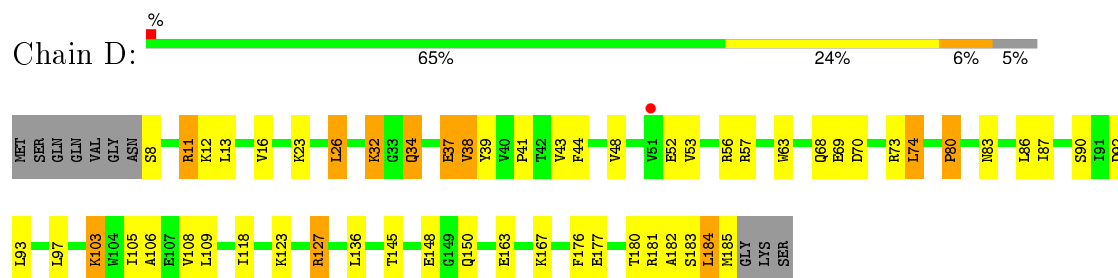




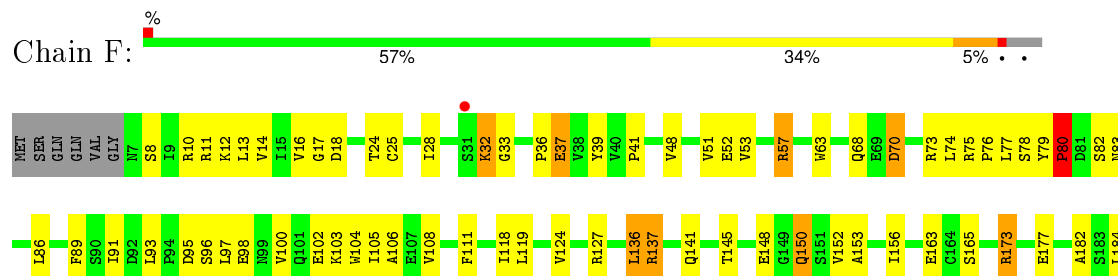
- Molecule 2: GTP-binding protein RHO1



- Molecule 2: GTP-binding protein RHO1



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.00Å 116.05Å 247.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.85 – 2.60 47.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.85-2.60) 99.6 (47.85-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.234 , 0.265 0.234 , 0.265	Depositor DCC
$R_{free}$ test set	2661 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.4	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 52811 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: PO4, MG, GNP

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	0.45	0/1556	0.67	0/2101
1	C	0.41	0/1518	0.65	0/2049
1	E	0.33	0/1406	0.59	0/1895
2	B	0.38	0/1409	0.64	0/1915
2	D	0.47	0/1409	0.69	0/1915
2	F	0.36	0/1430	0.61	0/1942
All	All	0.40	0/8728	0.64	0/11817

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

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	1522	0	1533	55	0
1	C	1485	0	1488	67	0
1	E	1377	0	1387	113	0
2	B	1385	0	1361	79	0
2	D	1385	0	1360	52	0
2	F	1406	0	1383	87	0
3	A	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	15	0	0	1	0
3	E	5	0	0	0	0
4	B	32	0	13	2	0
4	D	32	0	13	1	0
4	F	32	0	13	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	29	0	0	0	0
6	B	7	0	0	0	0
6	C	24	0	0	0	0
6	D	25	0	0	4	0
6	E	6	0	0	0	0
6	F	7	0	0	0	0
All	All	8792	0	8551	434	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 25.

All (434) 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)
2:D:34:GLN:HE21	2:D:34:GLN:HA	1.16	1.10
1:C:102:GLY:HA3	2:F:11:ARG:HH22	1.15	1.06
1:E:147:ASN:HD22	1:E:150:LEU:HG	1.16	1.03
1:E:112:VAL:HG11	1:E:209:PHE:HB2	1.41	1.02
2:B:97:LEU:HD11	2:B:152:VAL:HG21	1.40	1.00
1:E:75:SER:HB2	1:E:78:LEU:HD13	1.45	0.97
2:F:12:LYS:H	2:F:83:ASN:HD22	0.99	0.97
1:E:190:LEU:HB3	1:E:192:MSE:HE1	1.48	0.94
1:A:159:ASN:HD21	1:A:163:SER:HB3	1.31	0.94
1:E:120:PHE:HB2	1:E:125:PRO:HG3	1.47	0.94
1:A:146:ASN:H	1:A:146:ASN:HD22	0.96	0.94
1:A:151:ILE:HD11	1:A:172:LEU:HG	1.49	0.93
1:A:146:ASN:ND2	1:A:146:ASN:H	1.67	0.92
2:D:12:LYS:H	2:D:83:ASN:HD22	1.18	0.91
1:C:98:ASP:HB2	1:C:103:GLU:H	1.34	0.91
2:F:12:LYS:H	2:F:83:ASN:ND2	1.68	0.91
2:B:12:LYS:H	2:B:83:ASN:HD22	1.18	0.90
1:E:240:GLU:O	1:E:244:GLN:HG2	1.72	0.89
1:C:98:ASP:HB3	1:C:102:GLY:H	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:LYS:HB3	1:E:137:ARG:HH12	1.41	0.86
2:F:137:ARG:HH11	2:F:137:ARG:HB3	1.42	0.85
2:B:124:VAL:HG23	2:B:164:CYS:O	1.76	0.85
1:E:135:LYS:HB3	1:E:137:ARG:NH1	1.92	0.83
2:D:37:GLU:CD	2:D:37:GLU:H	1.82	0.83
2:D:34:GLN:NE2	2:D:34:GLN:HA	1.93	0.82
1:C:98:ASP:HB3	1:C:102:GLY:N	1.94	0.82
1:A:147:ASN:HD22	1:A:150:LEU:HG	1.45	0.82
2:F:12:LYS:N	2:F:83:ASN:HD22	1.78	0.81
1:E:147:ASN:ND2	1:E:150:LEU:HG	1.95	0.81
1:E:182:LEU:HD23	1:E:182:LEU:H	1.44	0.80
1:C:118:SER:HB3	1:C:135:LYS:HE3	1.63	0.80
1:C:216:LEU:O	1:C:220:THR:HG23	1.82	0.79
1:C:102:GLY:HA3	2:F:11:ARG:NH2	1.96	0.79
1:E:151:ILE:HG22	1:E:172:LEU:HB2	1.63	0.79
1:C:186:GLU:HG2	2:D:73:ARG:NH2	1.97	0.79
1:C:241:ARG:O	1:C:245:ARG:HG3	1.81	0.79
2:F:57:ARG:HB3	2:F:57:ARG:HH11	1.45	0.78
2:F:32:LYS:HG3	2:F:33:GLY:H	1.48	0.78
2:B:101:GLN:O	2:B:105:ILE:HD11	1.83	0.77
1:E:151:ILE:HG12	1:E:216:LEU:HD11	1.65	0.76
2:D:12:LYS:H	2:D:83:ASN:ND2	1.82	0.76
1:C:214:ILE:HD11	1:C:236:PHE:HB3	1.66	0.75
1:E:154:HIS:HB3	1:E:166:ILE:HD13	1.66	0.74
1:E:240:GLU:HB2	1:E:241:ARG:HE	1.52	0.74
1:A:240:GLU:O	1:A:244:GLN:HG2	1.86	0.74
2:F:97:LEU:HD21	2:F:152:VAL:HG21	1.70	0.72
1:E:184:ILE:HD12	1:E:197:TYR:OH	1.89	0.72
1:E:124:ARG:NH1	1:E:183:GLU:HB3	2.06	0.71
1:E:118:SER:HB2	1:E:135:LYS:HE3	1.74	0.70
2:F:37:GLU:CD	2:F:37:GLU:H	1.96	0.69
2:B:12:LYS:H	2:B:83:ASN:ND2	1.91	0.69
2:B:91:ILE:CD1	2:B:124:VAL:HA	2.23	0.69
1:E:178:VAL:HG12	1:E:231:TRP:HE1	1.57	0.68
1:A:105:PRO:O	1:A:145:PRO:HG3	1.93	0.68
1:A:151:ILE:HG13	1:A:172:LEU:HB2	1.74	0.68
2:D:145:THR:OG1	2:D:148:GLU:HG3	1.93	0.68
1:E:75:SER:HB2	1:E:78:LEU:CD1	2.21	0.68
1:E:217:TYR:CD2	1:E:226:PRO:HD3	2.29	0.68
1:E:110:THR:HG22	1:E:111:HIS:N	2.08	0.68
1:E:168:ARG:HH12	1:E:194:LYS:NZ	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:LYS:N	2:D:83:ASN:HD22	1.90	0.67
1:C:194:LYS:HB2	1:C:194:LYS:NZ	2.09	0.67
1:C:100:LYS:HD3	2:F:187:LYS:HZ2	1.59	0.67
1:C:168:ARG:HD2	1:C:169:THR:H	1.59	0.67
2:B:180:THR:O	2:B:184:LEU:HD13	1.95	0.67
2:D:127:ARG:HH22	2:D:163:GLU:CD	1.99	0.67
1:E:77:PHE:HE2	2:F:41:PRO:HG2	1.59	0.67
2:B:127:ARG:HH22	2:B:163:GLU:CD	1.98	0.67
2:B:105:ILE:HD12	2:B:106:ALA:H	1.59	0.66
2:B:91:ILE:HD13	2:B:124:VAL:HA	1.76	0.66
1:A:86:ARG:O	1:A:90:ILE:HG22	1.94	0.66
2:F:76:PRO:HB3	2:F:111:PHE:HE1	1.60	0.66
2:D:182:ALA:O	2:D:185:MET:HG2	1.95	0.65
1:E:179:GLU:HG3	1:E:229:VAL:HB	1.78	0.65
1:A:184:ILE:HG22	1:A:186:GLU:H	1.61	0.65
1:E:109:ILE:HG12	1:E:142:SER:HA	1.77	0.65
2:F:137:ARG:NH1	2:F:137:ARG:HB3	2.12	0.65
1:A:184:ILE:HD12	1:A:184:ILE:N	2.10	0.65
2:F:12:LYS:HE3	2:F:63:TRP:CE2	2.32	0.65
2:B:10:ARG:HG2	2:B:59:GLU:HB3	1.76	0.65
1:E:182:LEU:N	1:E:182:LEU:HD23	2.12	0.65
1:C:194:LYS:HB2	1:C:194:LYS:HZ3	1.62	0.65
2:F:76:PRO:HB3	2:F:111:PHE:CE1	2.32	0.65
1:E:243:TYR:O	1:E:247:VAL:HG13	1.97	0.64
1:A:247:VAL:HB	1:A:249:THR:HG22	1.79	0.64
2:B:87:ILE:HD11	2:B:108:VAL:HG21	1.80	0.64
1:C:101:THR:HG22	1:C:103:GLU:OE2	1.97	0.64
1:A:147:ASN:ND2	1:A:150:LEU:HG	2.10	0.63
1:A:101:THR:HB	1:A:103:GLU:OE2	1.98	0.63
2:B:100:VAL:O	2:B:105:ILE:HG13	1.98	0.63
1:A:146:ASN:ND2	1:A:146:ASN:N	2.43	0.63
2:F:124:VAL:HG12	2:F:165:SER:HB2	1.80	0.63
1:A:241:ARG:HD2	1:A:245:ARG:CZ	2.28	0.63
1:C:225:VAL:HG11	1:C:228:LEU:HD21	1.81	0.63
2:D:8:SER:HB2	2:D:57:ARG:O	1.99	0.63
1:E:217:TYR:CE2	1:E:226:PRO:HD3	2.33	0.63
1:E:78:LEU:H	1:E:78:LEU:HD12	1.64	0.63
1:A:146:ASN:N	1:A:146:ASN:HD22	1.81	0.63
2:B:105:ILE:CG2	2:B:156:ILE:HB	2.29	0.62
2:B:12:LYS:N	2:B:83:ASN:HD22	1.94	0.62
2:F:78:SER:C	2:F:80:PRO:HD2	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:LEU:HD13	1:C:226:PRO:HG2	1.81	0.62
1:E:137:ARG:HH11	1:E:137:ARG:HG2	1.65	0.62
2:B:101:GLN:C	2:B:105:ILE:HD11	2.20	0.62
1:E:106:ASN:ND2	1:E:145:PRO:HD3	2.14	0.62
2:F:73:ARG:HH11	2:F:74:LEU:HD11	1.64	0.62
1:C:105:PRO:O	1:C:145:PRO:HG3	1.99	0.62
2:B:37:GLU:CD	2:B:37:GLU:H	2.02	0.62
2:F:86:LEU:HD22	2:F:118:ILE:HB	1.82	0.62
2:F:182:ALA:HA	2:F:185:MET:SD	2.40	0.62
1:E:76:ASN:O	1:E:80:GLU:HG2	1.99	0.61
1:E:200:THR:HG21	1:E:206:ARG:HB2	1.82	0.61
2:B:90:SER:OG	2:B:92:ASP:OD1	2.19	0.61
2:F:105:ILE:HD13	2:F:156:ILE:HB	1.82	0.61
1:A:118:SER:HB3	1:A:135:LYS:HE2	1.83	0.61
1:E:175:LEU:HD21	1:E:178:VAL:HG23	1.82	0.61
1:C:214:ILE:HG12	1:C:236:PHE:CD1	2.35	0.61
1:E:177:ARG:HE	1:E:229:VAL:HG21	1.66	0.60
1:E:233:LEU:HB3	1:E:238:LEU:HD12	1.84	0.60
1:C:200:THR:CG2	1:C:202:SER:O	2.50	0.60
1:C:202:SER:HB2	2:D:70:ASP:HB3	1.83	0.59
1:A:200:THR:HG23	1:A:205:GLU:HB2	1.85	0.59
1:E:174:GLU:O	1:E:176:VAL:HG23	2.01	0.59
2:F:18:ASP:OD1	2:F:96:SER:HA	2.02	0.59
1:C:211:LYS:HD2	1:C:235:LEU:HD22	1.84	0.59
1:E:241:ARG:H	1:E:241:ARG:CD	2.15	0.59
2:F:73:ARG:HG3	2:F:74:LEU:HD22	1.83	0.59
1:C:100:LYS:HD3	2:F:187:LYS:NZ	2.18	0.58
1:C:98:ASP:CB	1:C:103:GLU:H	2.12	0.58
2:B:182:ALA:O	2:B:185:MET:HG2	2.04	0.58
1:E:110:THR:HG22	1:E:111:HIS:H	1.68	0.58
1:C:214:ILE:C	1:C:214:ILE:HD12	2.25	0.58
2:D:68:GLN:HG3	6:D:195:HOH:O	2.04	0.58
2:B:152:VAL:O	2:B:156:ILE:HG23	2.04	0.58
2:B:127:ARG:NH2	2:B:163:GLU:OE2	2.38	0.57
2:B:12:LYS:HE3	2:B:63:TRP:CE2	2.40	0.57
2:B:13:LEU:C	2:B:13:LEU:HD23	2.25	0.57
2:D:34:GLN:HE21	2:D:34:GLN:CA	1.98	0.56
1:C:201:ASN:O	2:D:73:ARG:NH2	2.38	0.56
2:F:97:LEU:CD1	2:F:152:VAL:HG11	2.35	0.56
1:A:120:PHE:HB2	1:A:125:PRO:HB3	1.86	0.56
2:B:58:VAL:HG21	2:B:180:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:HIS:HB3	1:E:166:ILE:CD1	2.36	0.56
1:E:78:LEU:N	1:E:78:LEU:HD12	2.21	0.56
2:B:57:ARG:HH11	2:B:57:ARG:HG3	1.70	0.56
2:F:145:THR:HG23	2:F:148:GLU:H	1.71	0.56
1:E:120:PHE:CE1	1:E:126:PRO:HD2	2.41	0.56
2:B:30:ASN:ND2	2:B:176:PHE:CD1	2.74	0.56
2:B:31:SER:O	2:B:32:LYS:HG2	2.06	0.56
2:F:91:ILE:HD12	2:F:124:VAL:HA	1.88	0.55
2:F:39:TYR:CZ	2:F:41:PRO:HG3	2.41	0.55
2:F:102:GLU:HA	2:F:102:GLU:OE1	2.06	0.55
1:A:151:ILE:CD1	1:A:172:LEU:HG	2.31	0.55
1:A:243:TYR:O	1:A:247:VAL:HG22	2.06	0.55
1:E:147:ASN:HD22	1:E:150:LEU:CG	2.06	0.55
2:F:57:ARG:NH1	2:F:57:ARG:HB3	2.17	0.55
1:A:200:THR:CG2	1:A:202:SER:O	2.55	0.55
2:F:127:ARG:HH22	2:F:163:GLU:CD	2.10	0.55
1:E:118:SER:CB	1:E:135:LYS:HE3	2.36	0.55
2:D:11:ARG:HA	2:D:83:ASN:ND2	2.21	0.54
1:E:124:ARG:NH1	1:E:183:GLU:CB	2.69	0.54
1:E:78:LEU:HD21	2:F:70:ASP:OD2	2.08	0.54
1:C:147:ASN:HB3	1:C:150:LEU:HG	1.88	0.54
2:B:58:VAL:HG21	2:B:180:THR:CG2	2.37	0.54
1:A:200:THR:CG2	1:A:205:GLU:HB2	2.37	0.54
2:F:86:LEU:CD2	2:F:118:ILE:HB	2.37	0.54
2:B:105:ILE:O	2:B:109:LEU:HG	2.07	0.54
1:E:131:LEU:HG	2:F:77:LEU:HB3	1.89	0.54
2:F:186:GLY:O	2:F:187:LYS:HB3	2.09	0.54
2:F:79:TYR:N	2:F:80:PRO:HD2	2.24	0.53
1:C:77:PHE:CZ	2:D:68:GLN:HG2	2.43	0.53
2:D:52:GLU:HA	2:D:52:GLU:OE1	2.07	0.53
2:B:98:GLU:HB3	2:B:102:GLU:OE1	2.09	0.53
1:E:166:ILE:HD12	1:E:167:GLY:N	2.23	0.53
1:A:77:PHE:CD2	2:B:41:PRO:HG2	2.44	0.53
1:A:76:ASN:O	1:A:80:GLU:HG2	2.09	0.53
2:B:73:ARG:HG2	2:B:74:LEU:HD22	1.91	0.53
1:E:120:PHE:CZ	1:E:126:PRO:HD2	2.44	0.53
1:A:171:GLN:O	1:A:174:GLU:HG3	2.09	0.53
2:F:73:ARG:NH1	2:F:74:LEU:HD11	2.24	0.53
2:B:171:GLY:O	2:B:175:VAL:HG23	2.08	0.53
2:B:8:SER:HB2	2:B:57:ARG:O	2.08	0.53
2:F:14:VAL:CG2	2:F:82:SER:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:THR:C	1:E:192:MSE:HE3	2.30	0.52
2:F:16:VAL:HG22	2:F:17:GLY:H	1.75	0.52
1:E:207:THR:O	1:E:211:LYS:HG3	2.09	0.52
2:B:45:GLU:HG2	2:B:47:TYR:CZ	2.44	0.52
2:B:16:VAL:C	2:B:23:LYS:HD3	2.30	0.52
1:E:138:LEU:HD12	1:E:138:LEU:N	2.25	0.52
2:B:118:ILE:CD1	2:B:179:ALA:HA	2.40	0.52
2:D:11:ARG:HG2	2:D:183:SER:OG	2.09	0.52
1:E:136:LYS:O	1:E:137:ARG:HD3	2.10	0.52
2:F:32:LYS:CG	2:F:33:GLY:H	2.21	0.52
1:E:110:THR:CG2	1:E:111:HIS:N	2.73	0.51
1:A:151:ILE:HD12	1:A:152:GLN:N	2.26	0.51
2:F:187:LYS:HB3	2:F:187:LYS:HZ3	1.76	0.51
1:E:75:SER:CB	1:E:78:LEU:HD13	2.30	0.51
1:E:244:GLN:O	1:E:247:VAL:HG22	2.11	0.51
2:B:105:ILE:CD1	2:B:106:ALA:H	2.23	0.51
1:E:217:TYR:CD2	1:E:225:VAL:HA	2.45	0.51
1:E:105:PRO:O	1:E:145:PRO:HG3	2.10	0.51
2:F:97:LEU:HD11	2:F:152:VAL:HG11	1.92	0.51
1:A:101:THR:O	1:A:103:GLU:HG2	2.11	0.51
1:C:186:GLU:HG2	2:D:73:ARG:CZ	2.39	0.51
1:E:141:LEU:CD2	1:E:153:ILE:HG12	2.40	0.51
1:E:114:ILE:HD11	1:E:137:ARG:HB2	1.93	0.51
1:E:137:ARG:NH2	1:E:157:ARG:HH11	2.09	0.51
2:F:8:SER:HB2	2:F:57:ARG:O	2.12	0.50
2:D:11:ARG:HD3	2:D:184:LEU:HD13	1.93	0.50
1:E:225:VAL:HG22	1:E:228:LEU:HD11	1.94	0.50
1:C:99:HIS:O	1:C:100:LYS:HG3	2.11	0.50
2:F:24:THR:O	2:F:28:ILE:HG12	2.11	0.50
2:B:104:TRP:O	2:B:108:VAL:HG23	2.11	0.50
1:C:194:LYS:CB	1:C:194:LYS:HZ3	2.24	0.50
2:B:78:SER:C	2:B:80:PRO:HD2	2.31	0.50
2:B:105:ILE:HG21	2:B:156:ILE:HB	1.92	0.50
2:F:79:TYR:N	2:F:80:PRO:CD	2.74	0.50
1:C:158:GLU:HB2	1:C:164:PHE:CE2	2.47	0.50
2:B:97:LEU:HD12	2:B:100:VAL:HG21	1.93	0.49
2:F:13:LEU:HD23	2:F:13:LEU:C	2.32	0.49
1:E:210:ILE:O	1:E:214:ILE:HG12	2.13	0.49
1:C:174:GLU:O	1:C:176:VAL:HG23	2.13	0.49
1:E:178:VAL:HG12	1:E:231:TRP:NE1	2.25	0.49
1:E:136:LYS:NZ	1:E:136:LYS:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:ALA:HA	2:D:185:MET:CE	2.43	0.49
1:E:160:SER:O	1:E:161:ASP:CG	2.51	0.49
2:D:37:GLU:HG2	2:D:38:VAL:HG12	1.93	0.49
1:C:168:ARG:HD2	1:C:169:THR:N	2.27	0.49
2:D:167:LYS:HE2	6:D:202:HOH:O	2.13	0.49
2:F:68:GLN:HA	2:F:68:GLN:NE2	2.28	0.49
1:E:217:TYR:CE2	1:E:225:VAL:HA	2.47	0.49
1:A:166:ILE:O	1:A:166:ILE:HG13	2.11	0.49
2:B:15:ILE:HG12	2:B:23:LYS:HD2	1.95	0.48
2:F:150:GLN:HE21	2:F:150:GLN:CA	2.26	0.48
1:E:185:SER:HB2	1:E:186:GLU:OE2	2.13	0.48
2:B:101:GLN:HA	2:B:105:ILE:CG1	2.43	0.48
2:D:105:ILE:HG23	2:D:106:ALA:N	2.28	0.48
1:E:77:PHE:HE2	2:F:41:PRO:CG	2.26	0.48
1:C:228:LEU:HD22	1:C:243:TYR:CE1	2.47	0.48
1:E:133:ASN:N	1:E:133:ASN:HD22	2.11	0.48
2:D:43:VAL:HG12	2:D:44:PHE:HD1	1.78	0.48
1:A:159:ASN:HD21	1:A:163:SER:CB	2.16	0.48
1:E:112:VAL:HG11	1:E:209:PHE:CB	2.28	0.48
2:F:16:VAL:HG22	2:F:17:GLY:N	2.28	0.48
2:F:11:ARG:HD2	2:F:184:LEU:HD23	1.94	0.48
1:A:151:ILE:HD12	1:A:151:ILE:C	2.33	0.48
1:A:200:THR:HG21	1:A:206:ARG:N	2.29	0.48
2:D:39:TYR:CZ	2:D:41:PRO:HG3	2.49	0.48
1:A:180:LYS:HB2	1:A:231:TRP:CE2	2.49	0.48
2:D:13:LEU:HD23	2:D:13:LEU:C	2.34	0.48
1:E:184:ILE:HD13	1:E:199:GLU:OE1	2.14	0.47
2:F:89:PHE:CG	2:F:97:LEU:HD23	2.49	0.47
1:E:110:THR:CG2	1:E:111:HIS:H	2.26	0.47
1:A:209:PHE:O	1:A:212:SER:HB2	2.15	0.47
1:C:159:ASN:C	1:C:160:SER:O	2.52	0.47
1:E:200:THR:CG2	1:E:206:ARG:HB2	2.44	0.47
2:F:96:SER:O	2:F:100:VAL:HG23	2.14	0.47
1:E:137:ARG:NH2	1:E:157:ARG:NH1	2.62	0.47
2:D:69:GLU:N	6:D:195:HOH:O	2.48	0.47
1:A:258:ILE:C	1:A:258:ILE:HD12	2.35	0.47
2:D:16:VAL:C	2:D:23:LYS:HD3	2.35	0.47
1:C:151:ILE:HD12	1:C:151:ILE:N	2.30	0.47
1:E:114:ILE:HD12	1:E:114:ILE:O	2.15	0.47
2:F:13:LEU:HD23	2:F:14:VAL:N	2.30	0.47
1:A:158:GLU:HB2	1:A:164:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:THR:O	2:D:184:LEU:HD22	2.15	0.47
2:D:145:THR:HG23	2:D:148:GLU:OE2	2.15	0.47
2:F:14:VAL:HG23	2:F:82:SER:HB3	1.96	0.47
2:B:118:ILE:HD11	2:B:179:ALA:HA	1.97	0.47
2:B:95:ASP:OD2	2:B:95:ASP:N	2.48	0.46
1:E:120:PHE:CD1	1:E:125:PRO:HB3	2.50	0.46
2:F:105:ILE:HG23	2:F:106:ALA:N	2.31	0.46
1:C:200:THR:HG21	1:C:206:ARG:N	2.31	0.46
1:C:86:ARG:HG3	1:C:108:TYR:CE2	2.50	0.46
2:B:105:ILE:HG23	2:B:156:ILE:HB	1.97	0.46
1:C:194:LYS:CB	1:C:194:LYS:NZ	2.77	0.46
1:E:147:ASN:HD21	1:E:149:LYS:HB2	1.80	0.46
2:D:182:ALA:HA	2:D:185:MET:HE3	1.96	0.46
1:A:241:ARG:HD2	1:A:245:ARG:NH2	2.31	0.46
2:B:79:TYR:N	2:B:80:PRO:HD2	2.31	0.46
1:E:85:ASP:O	1:E:89:ILE:HG13	2.15	0.46
2:B:91:ILE:HD11	2:B:124:VAL:HA	1.96	0.46
2:F:95:ASP:O	2:F:98:GLU:HB2	2.16	0.46
1:E:175:LEU:HG	1:E:192:MSE:HE2	1.98	0.46
1:E:178:VAL:HG22	1:E:190:LEU:CD2	2.46	0.46
2:B:12:LYS:HE3	2:B:63:TRP:CD2	2.51	0.46
1:E:182:LEU:CD2	1:E:182:LEU:H	2.21	0.46
1:C:200:THR:HG21	1:C:202:SER:O	2.15	0.46
1:C:146:ASN:H	1:C:146:ASN:ND2	2.12	0.46
2:B:12:LYS:HD3	2:B:81:ASP:O	2.16	0.45
2:D:127:ARG:NH2	2:D:163:GLU:OE2	2.48	0.45
1:A:142:SER:OG	1:A:154:HIS:NE2	2.45	0.45
1:C:110:THR:HG22	1:C:141:LEU:HD12	1.97	0.45
2:B:14:VAL:HG21	2:B:82:SER:OG	2.17	0.45
1:E:81:GLN:HE22	1:E:84:ARG:HD3	1.81	0.45
2:D:74:LEU:HD22	2:D:74:LEU:H	1.82	0.45
1:A:81:GLN:OE1	1:A:84:ARG:NH1	2.50	0.45
2:D:177:GLU:O	2:D:181:ARG:HG3	2.17	0.45
2:B:19:GLY:O	2:B:20:ALA:HB3	2.16	0.45
2:F:186:GLY:O	2:F:187:LYS:CB	2.64	0.45
1:A:183:GLU:HB2	1:A:184:ILE:HD12	1.98	0.45
1:C:86:ARG:HG3	1:C:108:TYR:CZ	2.52	0.45
1:E:218:ILE:HG23	1:E:223:GLY:HA2	1.99	0.45
1:E:137:ARG:NH1	1:E:137:ARG:HG2	2.31	0.45
1:E:239:ASP:OD2	1:E:241:ARG:HG2	2.16	0.45
1:E:225:VAL:CG2	1:E:228:LEU:HD11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:152:VAL:O	2:F:156:ILE:HG12	2.17	0.45
2:D:53:VAL:HG21	2:D:180:THR:HG22	1.99	0.45
2:F:119:LEU:HD23	2:F:153:ALA:HB2	1.99	0.45
1:A:106:ASN:ND2	1:A:145:PRO:HD3	2.32	0.45
1:E:229:VAL:HG12	1:E:230:ASN:ND2	2.32	0.45
1:A:98:ASP:OD2	1:A:100:LYS:HB2	2.17	0.45
2:B:87:ILE:HG21	2:B:100:VAL:HG13	1.99	0.44
2:F:12:LYS:HE3	2:F:63:TRP:CD2	2.52	0.44
2:F:145:THR:HG22	2:F:148:GLU:CD	2.36	0.44
2:D:68:GLN:HB2	6:D:194:HOH:O	2.16	0.44
1:A:137:ARG:HH11	1:A:137:ARG:HG2	1.82	0.44
1:C:224:HIS:CE1	1:C:251:ARG:HD3	2.52	0.44
2:F:11:ARG:HH11	2:F:11:ARG:HG2	1.83	0.44
2:B:96:SER:O	2:B:100:VAL:HG23	2.18	0.44
1:E:190:LEU:CB	1:E:192:MSE:HE1	2.34	0.44
1:E:120:PHE:CZ	1:E:126:PRO:CD	3.00	0.44
2:F:39:TYR:CE2	2:F:41:PRO:HG3	2.52	0.44
2:B:79:TYR:N	2:B:80:PRO:CD	2.80	0.44
1:E:111:HIS:O	1:E:112:VAL:HG13	2.17	0.44
2:D:11:ARG:HA	2:D:83:ASN:HD22	1.83	0.44
1:E:168:ARG:HH12	1:E:194:LYS:CE	2.30	0.44
2:F:104:TRP:O	2:F:108:VAL:HG23	2.17	0.44
2:B:39:TYR:CZ	2:B:41:PRO:HG3	2.53	0.44
1:C:202:SER:OG	1:C:205:GLU:HG3	2.18	0.44
1:C:192:MSE:HG2	1:C:196:TYR:HE1	1.82	0.44
2:F:111:PHE:N	2:F:111:PHE:CD2	2.86	0.44
1:A:124:ARG:HE	1:A:184:ILE:CD1	2.29	0.44
1:C:77:PHE:CD2	2:D:41:PRO:HG2	2.53	0.44
2:B:42:THR:HB	4:B:301:GNP:O2G	2.18	0.44
2:B:91:ILE:CD1	2:B:127:ARG:HB2	2.48	0.43
1:E:238:LEU:HB2	1:E:242:SER:HB2	1.99	0.43
1:C:224:HIS:ND1	1:C:251:ARG:HD3	2.33	0.43
1:A:101:THR:O	1:A:103:GLU:N	2.51	0.43
2:B:13:LEU:HD23	2:B:14:VAL:N	2.33	0.43
2:B:123:LYS:HG2	4:B:301:GNP:C6	2.47	0.43
2:B:91:ILE:HD12	2:B:127:ARG:HB2	1.99	0.43
1:E:151:ILE:HG21	1:E:172:LEU:HD22	2.00	0.43
2:B:86:LEU:HD22	2:B:118:ILE:HB	2.00	0.43
1:E:178:VAL:HG22	1:E:190:LEU:HD22	2.01	0.43
1:A:159:ASN:ND2	1:A:163:SER:HB3	2.15	0.43
1:A:157:ARG:HH21	3:A:323:PO4:P	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:ARG:O	1:E:165:GLN:HG2	2.18	0.43
1:C:100:LYS:HE2	2:F:187:LYS:HB2	2.01	0.43
1:C:174:GLU:O	1:C:192:MSE:HA	2.18	0.43
2:F:136:LEU:HA	2:F:136:LEU:HD12	1.86	0.43
2:B:97:LEU:HA	2:B:100:VAL:HG23	2.00	0.43
1:E:114:ILE:CD1	1:E:137:ARG:HB2	2.47	0.43
2:F:73:ARG:HE	2:F:74:LEU:HD21	1.83	0.43
1:A:200:THR:HG21	1:A:202:SER:O	2.19	0.43
1:C:160:SER:C	1:C:162:GLY:H	2.21	0.43
2:F:136:LEU:HB3	2:F:141:GLN:O	2.19	0.43
1:C:228:LEU:HD22	1:C:243:TYR:HE1	1.84	0.43
2:F:25:CYS:SG	2:F:36:PRO:HD2	2.59	0.43
2:F:74:LEU:HD22	2:F:74:LEU:H	1.84	0.42
2:F:150:GLN:NE2	2:F:150:GLN:CA	2.81	0.42
2:B:28:ILE:CD1	2:B:36:PRO:HG2	2.49	0.42
1:E:78:LEU:CD1	1:E:78:LEU:H	2.30	0.42
2:B:50:ASP:OD1	2:B:59:GLU:HA	2.20	0.42
1:A:141:LEU:CD2	1:A:153:ILE:HG12	2.49	0.42
2:F:16:VAL:HG22	2:F:104:TRP:CZ3	2.54	0.42
1:C:202:SER:CB	2:D:70:ASP:HB3	2.49	0.42
2:D:48:VAL:O	2:D:48:VAL:HG23	2.19	0.42
1:E:78:LEU:HD11	2:F:70:ASP:OD2	2.19	0.42
1:C:184:ILE:HG22	1:C:186:GLU:OE1	2.20	0.42
2:F:119:LEU:CD2	2:F:152:VAL:HG23	2.50	0.42
2:F:75:ARG:HB3	2:F:76:PRO:HD3	2.01	0.42
2:D:43:VAL:HG12	2:D:44:PHE:CD1	2.55	0.42
1:A:202:SER:OG	1:A:205:GLU:HG3	2.19	0.42
2:D:74:LEU:N	2:D:74:LEU:HD13	2.34	0.42
2:B:119:LEU:CD2	2:B:152:VAL:HG23	2.50	0.42
2:F:16:VAL:CG2	2:F:104:TRP:CZ3	3.03	0.42
1:E:106:ASN:HB3	1:E:143:ALA:O	2.20	0.42
1:E:133:ASN:N	1:E:133:ASN:ND2	2.67	0.42
2:B:124:VAL:HG23	2:B:164:CYS:C	2.37	0.42
1:E:158:GLU:HB2	1:E:164:PHE:CE2	2.55	0.42
1:C:159:ASN:O	1:C:160:SER:O	2.38	0.42
2:D:87:ILE:HD11	2:D:108:VAL:HG21	2.02	0.42
1:C:97:PRO:HA	1:C:103:GLU:O	2.19	0.41
1:E:243:TYR:CE1	1:E:247:VAL:HG12	2.54	0.41
1:A:244:GLN:OE1	1:A:244:GLN:HA	2.20	0.41
2:B:10:ARG:HD3	2:B:59:GLU:OE1	2.20	0.41
1:E:215:THR:O	1:E:219:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LEU:O	1:C:134:LYS:HG2	2.20	0.41
1:E:194:LYS:HE3	1:E:196:TYR:OH	2.20	0.41
2:F:127:ARG:NH2	2:F:163:GLU:OE2	2.53	0.41
1:C:160:SER:O	1:C:162:GLY:N	2.52	0.41
1:A:201:ASN:HB3	2:B:71:TYR:CE1	2.55	0.41
1:E:126:PRO:HA	1:E:127:PRO:HD3	1.93	0.41
2:F:53:VAL:O	2:F:53:VAL:HG23	2.21	0.41
2:B:11:ARG:HA	2:B:83:ASN:ND2	2.36	0.41
1:E:229:VAL:O	1:E:230:ASN:HB2	2.21	0.41
2:F:51:VAL:HG12	2:F:52:GLU:N	2.35	0.41
1:C:247:VAL:C	1:C:249:THR:H	2.23	0.41
1:C:99:HIS:O	1:C:100:LYS:CG	2.68	0.41
2:F:48:VAL:HG23	2:F:48:VAL:O	2.20	0.41
2:D:26:LEU:HD22	2:D:176:PHE:HE1	1.86	0.41
1:E:168:ARG:HH12	1:E:194:LYS:HZ3	1.68	0.41
1:E:161:ASP:OD1	1:E:163:SER:HB2	2.21	0.41
1:E:170:TRP:CD1	1:E:192:MSE:HG2	2.55	0.41
2:D:26:LEU:HD22	2:D:176:PHE:CE1	2.56	0.41
2:B:54:ASP:OD1	2:B:181:ARG:NH1	2.54	0.41
2:B:69:GLU:O	2:B:72:ASP:OD2	2.39	0.41
1:C:168:ARG:HH12	3:C:321:PO4:P	2.44	0.41
1:A:108:TYR:CZ	1:A:110:THR:HA	2.56	0.41
2:B:149:GLY:O	2:B:152:VAL:HG22	2.21	0.41
1:E:177:ARG:NH2	1:E:179:GLU:OE2	2.54	0.41
2:F:73:ARG:HE	2:F:74:LEU:CD2	2.33	0.41
1:C:87:LYS:O	1:C:91:ASN:HB2	2.21	0.41
2:D:123:LYS:HG2	4:D:301:GNP:C6	2.51	0.41
1:C:237:TYR:O	1:C:238:LEU:HD12	2.20	0.41
2:F:16:VAL:CG2	2:F:75:ARG:HD2	2.51	0.41
1:E:200:THR:OG1	1:E:205:GLU:HB3	2.21	0.41
1:C:200:THR:HG23	1:C:205:GLU:HB2	2.03	0.41
2:B:95:ASP:O	2:B:98:GLU:HB2	2.21	0.41
2:B:15:ILE:HD11	2:B:88:CYS:SG	2.61	0.41
2:D:86:LEU:HD22	2:D:118:ILE:HB	2.03	0.41
2:D:90:SER:OG	2:D:92:ASP:OD1	2.35	0.41
2:B:28:ILE:HD12	2:B:36:PRO:HG2	2.02	0.40
1:A:259:LYS:HD3	1:A:259:LYS:HA	1.89	0.40
2:F:97:LEU:HD13	2:F:152:VAL:HG11	2.04	0.40
2:B:162:TYR:CD1	2:B:162:TYR:N	2.89	0.40
2:B:27:LEU:HD22	2:B:62:LEU:HD13	2.04	0.40
2:D:109:LEU:HA	2:D:109:LEU:HD23	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:173:ARG:O	2:F:177:GLU:HG3	2.20	0.40
1:E:94:PHE:HA	1:E:105:PRO:HB2	2.04	0.40
2:D:12:LYS:HE3	2:D:63:TRP:CD2	2.57	0.40
1:C:146:ASN:HD22	1:C:146:ASN:H	1.69	0.40
1:C:229:VAL:O	1:C:230:ASN:HB2	2.21	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	183/320 (57%)	172 (94%)	9 (5%)	2 (1%)	17	36
1	C	178/320 (56%)	161 (90%)	12 (7%)	5 (3%)	6	10
1	E	162/320 (51%)	144 (89%)	17 (10%)	1 (1%)	30	56
2	B	176/188 (94%)	166 (94%)	7 (4%)	3 (2%)	11	22
2	D	176/188 (94%)	167 (95%)	6 (3%)	3 (2%)	11	22
2	F	179/188 (95%)	166 (93%)	9 (5%)	4 (2%)	8	15
All	All	1054/1524 (69%)	976 (93%)	60 (6%)	18 (2%)	11	22

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	80	PRO
1	C	97	PRO
2	D	80	PRO
2	F	80	PRO
1	C	160	SER
1	C	161	ASP
2	D	32	LYS

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Mol	Chain	Res	Type
2	F	186	GLY
2	B	32	LYS
2	B	103	LYS
1	C	252	PRO
2	D	103	LYS
1	E	160	SER
2	F	32	LYS
2	F	103	LYS
1	A	160	SER
1	C	253	GLY
1	A	102	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	172/290 (59%)	159 (92%)	13 (8%)	16	32
1	C	167/290 (58%)	151 (90%)	16 (10%)	10	20
1	E	155/290 (53%)	148 (96%)	7 (4%)	34	62
2	B	153/161 (95%)	145 (95%)	8 (5%)	29	54
2	D	153/161 (95%)	137 (90%)	16 (10%)	8	16
2	F	155/161 (96%)	144 (93%)	11 (7%)	18	36
All	All	955/1353 (71%)	884 (93%)	71 (7%)	17	34

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ILE
1	A	140	ILE
1	A	146	ASN
1	A	151	ILE
1	A	159	ASN
1	A	161	ASP
1	A	172	LEU

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Mol	Chain	Res	Type
1	A	175	LEU
1	A	192	MSE
1	A	193	SER
1	A	200	THR
1	A	228	LEU
1	A	247	VAL
2	B	37	GLU
2	B	57	ARG
2	B	80	PRO
2	B	95	ASP
2	B	105	ILE
2	B	146	SER
2	B	150	GLN
2	B	159	THR
1	C	91	ASN
1	C	96	ARG
1	C	171	GLN
1	C	172	LEU
1	C	175	LEU
1	C	182	LEU
1	C	183	GLU
1	C	192	MSE
1	C	200	THR
1	C	207	THR
1	C	212	SER
1	C	214	ILE
1	C	216	LEU
1	C	220	THR
1	C	228	LEU
1	C	247	VAL
2	D	11	ARG
2	D	26	LEU
2	D	32	LYS
2	D	34	GLN
2	D	37	GLU
2	D	38	VAL
2	D	56	ARG
2	D	74	LEU
2	D	80	PRO
2	D	93	LEU
2	D	97	LEU
2	D	103	LYS

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Mol	Chain	Res	Type
2	D	127	ARG
2	D	136	LEU
2	D	150	GLN
2	D	184	LEU
1	E	104	PRO
1	E	138	LEU
1	E	175	LEU
1	E	182	LEU
1	E	192	MSE
1	E	222	GLU
1	E	241	ARG
2	F	10	ARG
2	F	37	GLU
2	F	57	ARG
2	F	70	ASP
2	F	80	PRO
2	F	93	LEU
2	F	136	LEU
2	F	137	ARG
2	F	150	GLN
2	F	173	ARG
2	F	187	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	107	ASN
1	A	133	ASN
1	A	146	ASN
1	A	147	ASN
1	A	152	GLN
1	A	159	ASN
1	A	171	GLN
2	B	30	ASN
2	B	68	GLN
2	B	83	ASN
2	B	101	GLN
2	B	141	GLN
2	B	150	GLN
2	B	155	GLN
1	C	106	ASN

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Mol	Chain	Res	Type
1	C	146	ASN
1	C	152	GLN
1	C	165	GLN
1	C	171	GLN
2	D	34	GLN
2	D	83	ASN
2	D	135	GLN
2	D	141	GLN
2	D	142	GLN
2	D	147	GLN
2	D	150	GLN
1	E	106	ASN
1	E	147	ASN
1	E	152	GLN
1	E	201	ASN
1	E	230	ASN
2	F	68	GLN
2	F	83	ASN
2	F	101	GLN
2	F	141	GLN
2	F	142	GLN
2	F	150	GLN
2	F	155	GLN

### 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 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	PO4	A	321	-	4,4,4	1.10	0	6,6,6	0.27	0
3	PO4	A	322	-	4,4,4	1.11	0	6,6,6	0.27	0
3	PO4	A	323	-	4,4,4	1.09	0	6,6,6	0.27	0
4	GNP	B	301	5	28,34,34	1.82	6 (21%)	33,54,54	2.31	10 (30%)
3	PO4	C	321	-	4,4,4	1.09	0	6,6,6	0.27	0
3	PO4	C	322	-	4,4,4	1.13	0	6,6,6	0.27	0
3	PO4	C	323	-	4,4,4	1.14	0	6,6,6	0.27	0
4	GNP	D	301	5	28,34,34	1.81	7 (25%)	33,54,54	2.26	8 (24%)
3	PO4	E	321	-	4,4,4	1.08	0	6,6,6	0.27	0
4	GNP	F	301	5	28,34,34	2.09	9 (32%)	33,54,54	2.33	10 (30%)

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	PO4	A	321	-	-	0/0/0/0	0/0/0/0
3	PO4	A	322	-	-	0/0/0/0	0/0/0/0
3	PO4	A	323	-	-	0/0/0/0	0/0/0/0
4	GNP	B	301	5	-	0/12/38/38	0/3/3/3
3	PO4	C	321	-	-	0/0/0/0	0/0/0/0
3	PO4	C	322	-	-	0/0/0/0	0/0/0/0
3	PO4	C	323	-	-	0/0/0/0	0/0/0/0
4	GNP	D	301	5	-	0/12/38/38	0/3/3/3
3	PO4	E	321	-	-	0/0/0/0	0/0/0/0
4	GNP	F	301	5	-	0/12/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	301	GNP	PB-O3A	-5.56	1.52	1.59
4	B	301	GNP	PB-O3A	-3.49	1.54	1.59
4	D	301	GNP	PB-O2B	-3.10	1.48	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	GNP	PB-O3A	-2.99	1.55	1.59
4	B	301	GNP	PB-O2B	-2.96	1.48	1.56
4	F	301	GNP	PB-O2B	-2.66	1.49	1.56
4	D	301	GNP	PG-O3G	-2.34	1.50	1.56
4	B	301	GNP	PG-O3G	-2.33	1.50	1.56
4	F	301	GNP	C8-N7	-2.15	1.30	1.34
4	F	301	GNP	PG-O3G	-2.08	1.50	1.56
4	D	301	GNP	PB-O1B	2.07	1.48	1.46
4	B	301	GNP	C2-N1	2.27	1.39	1.35
4	F	301	GNP	PB-O1B	2.28	1.48	1.46
4	F	301	GNP	C4-N3	2.29	1.39	1.35
4	F	301	GNP	C2-N1	2.67	1.40	1.35
4	D	301	GNP	C2-N1	2.82	1.40	1.35
4	D	301	GNP	PG-O1G	4.04	1.50	1.46
4	B	301	GNP	PG-O1G	4.23	1.50	1.46
4	D	301	GNP	C6-N1	4.72	1.41	1.33
4	F	301	GNP	PG-O1G	4.77	1.51	1.46
4	F	301	GNP	C6-N1	4.85	1.42	1.33
4	B	301	GNP	C6-N1	4.99	1.42	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	GNP	C5-C6-N1	-7.99	112.67	123.59
4	D	301	GNP	C5-C6-N1	-7.92	112.76	123.59
4	F	301	GNP	C5-C6-N1	-7.69	113.08	123.59
4	B	301	GNP	O3G-PG-O1G	-3.99	102.89	113.49
4	F	301	GNP	O3G-PG-O1G	-3.70	103.65	113.49
4	D	301	GNP	O3G-PG-O1G	-3.57	104.01	113.49
4	F	301	GNP	N3-C2-N1	-3.11	122.71	127.44
4	D	301	GNP	N3-C2-N1	-3.03	122.83	127.44
4	B	301	GNP	N3-C2-N1	-2.85	123.10	127.44
4	F	301	GNP	PA-O3A-PB	-2.75	123.45	132.67
4	D	301	GNP	O1B-PB-N3B	-2.30	108.38	111.90
4	F	301	GNP	O1B-PB-N3B	-2.17	108.57	111.90
4	B	301	GNP	C6-C5-C4	-2.06	118.44	120.90
4	D	301	GNP	C6-C5-C4	-2.06	118.44	120.90
4	F	301	GNP	C6-C5-C4	-2.03	118.47	120.90
4	B	301	GNP	PA-O3A-PB	-2.01	125.94	132.67
4	B	301	GNP	O4'-C1'-N9	2.09	112.48	108.10
4	B	301	GNP	O3A-PA-O5'	2.14	108.61	102.94
4	B	301	GNP	O3G-PG-O2G	2.31	114.42	107.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	301	GNP	O3A-PA-O5'	2.45	109.44	102.94
4	D	301	GNP	O2B-PB-O1B	2.52	115.26	110.00
4	F	301	GNP	O4'-C1'-N9	2.53	113.40	108.10
4	D	301	GNP	O4'-C1'-N9	2.64	113.64	108.10
4	B	301	GNP	O2B-PB-O1B	2.93	116.11	110.00
4	F	301	GNP	O2B-PB-O1B	3.51	117.32	110.00
4	D	301	GNP	C6-N1-C2	6.18	124.51	115.94
4	B	301	GNP	C6-N1-C2	6.19	124.52	115.94
4	F	301	GNP	C6-N1-C2	6.22	124.57	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	323	PO4	1	0
4	B	301	GNP	2	0
3	C	321	PO4	1	0
4	D	301	GNP	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	184/320 (57%)	0.11	6 (3%) 50 43	31, 53, 84, 119	0
1	C	179/320 (55%)	-0.06	0 100 100	36, 57, 97, 123	0
1	E	165/320 (51%)	1.21	30 (18%) 2 1	72, 108, 129, 133	0
2	B	178/188 (94%)	0.68	15 (8%) 14 9	52, 74, 97, 108	0
2	D	178/188 (94%)	0.32	1 (0%) 90 88	34, 47, 78, 99	0
2	F	181/188 (96%)	0.34	2 (1%) 82 79	51, 76, 95, 108	0
All	All	1065/1524 (69%)	0.42	54 (5%) 32 25	31, 67, 116, 133	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	150	LEU	6.1
1	E	164	PHE	4.9
2	B	31	SER	4.8
1	E	170	TRP	4.8
1	E	162	GLY	4.7
1	E	147	ASN	4.6
1	E	128	ASP	4.3
1	E	144	LYS	4.3
1	E	172	LEU	4.2
1	E	146	ASN	4.0
2	B	57	ARG	4.0
1	E	94	PHE	3.8
1	E	195	LYS	3.8
1	A	260	SER	3.8
1	E	154	HIS	3.7
1	E	182	LEU	3.6
1	E	140	ILE	3.6
2	B	152	VAL	3.5
1	A	101	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	148	ALA	3.4
1	E	175	LEU	3.3
1	E	153	ILE	3.3
1	E	119	LYS	3.1
1	E	104	PRO	3.0
1	E	155	LYS	2.9
2	B	139	GLU	2.9
1	E	105	PRO	2.8
1	E	190	LEU	2.8
1	E	228	LEU	2.7
2	B	50	ASP	2.6
1	E	133	ASN	2.6
2	D	51	VAL	2.5
1	A	99	HIS	2.5
1	E	156	ALA	2.5
1	A	161	ASP	2.5
1	E	168	ARG	2.4
1	A	241	ARG	2.4
2	B	32	LYS	2.4
1	E	149	LYS	2.4
2	F	31	SER	2.4
2	B	156	ILE	2.3
2	B	184	LEU	2.3
2	B	56	ARG	2.3
2	B	9	ILE	2.3
2	F	187	LYS	2.2
1	E	230	ASN	2.2
2	B	49	ALA	2.2
2	B	51	VAL	2.1
2	B	138	GLN	2.1
1	E	141	LEU	2.1
2	B	135	GLN	2.0
1	E	178	VAL	2.0
1	A	166	ILE	2.0
2	B	102	GLU	2.0

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

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(Å <sup>2</sup> )	Q<0.9
4	GNP	D	301	32/32	0.98	0.20	0.45	27,34,39,42	0
4	GNP	F	301	32/32	0.97	0.18	0.08	58,62,65,68	0
4	GNP	B	301	32/32	0.98	0.15	-0.97	49,57,60,61	0
5	MG	D	401	1/1	0.96	0.16	-1.21	38,38,38,38	0
5	MG	B	401	1/1	0.97	0.12	-2.43	46,46,46,46	0
5	MG	F	401	1/1	0.88	0.11	-4.02	57,57,57,57	0
3	PO4	A	323	5/5	0.82	0.24	-	110,110,111,111	0
3	PO4	C	321	5/5	0.97	0.10	-	71,72,72,73	0
3	PO4	A	322	5/5	0.96	0.18	-	82,83,83,84	0
3	PO4	C	322	5/5	0.94	0.14	-	67,67,68,70	0
3	PO4	C	323	5/5	0.96	0.18	-	93,94,95,95	0
3	PO4	E	321	5/5	0.53	0.27	-	146,147,147,147	0
3	PO4	A	321	5/5	0.87	0.17	-	109,110,110,110	0

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

There are no such residues in this entry.