



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2016 – 12:09 AM EST

PDB ID : 5K1I  
Title : PDE4 crystal structure in complex with small molecule inhibitor  
Authors : Segarra, V.; Hernandez, B.; Ferrer-Miralles, N.; Korndorfer, I.; Aymami, J.  
Deposited on : 2016-05-18  
Resolution : 2.61 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

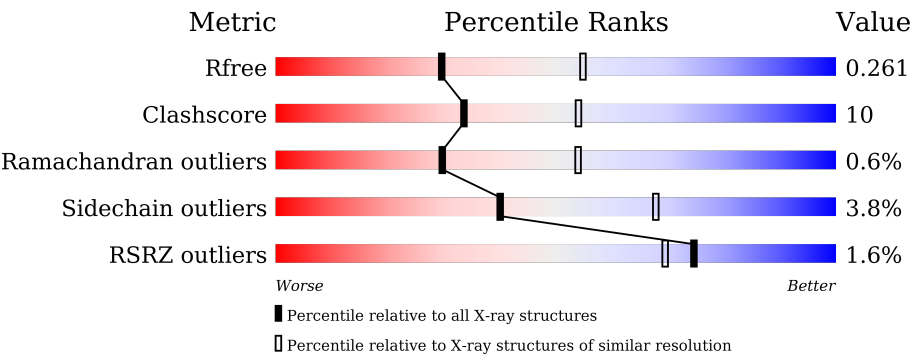
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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	326	<div><div>2%</div><div><div></div><div>73%</div><div>23%</div><div>..</div></div></div>
1	B	326	<div><div>%</div><div><div></div><div>77%</div><div>21%</div><div>.</div></div></div>
1	C	326	<div><div>%</div><div><div></div><div>77%</div><div>20%</div><div>..</div></div></div>
1	D	326	<div><div>%</div><div><div></div><div>80%</div><div>18%</div><div>.</div></div></div>
1	E	326	<div><div>%</div><div><div></div><div>83%</div><div>15%</div><div>..</div></div></div>
1	F	326	<div><div>4%</div><div><div></div><div>70%</div><div>27%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	326	
1	H	326	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	6PT	D	1001	-	-	-	X
2	6PT	G	1001	-	-	-	X
4	MG	A	1003	-	-	-	X
4	MG	B	1003	-	-	-	X
4	MG	C	1003	-	-	-	X
4	MG	D	1003	-	-	-	X
4	MG	E	1003	-	-	-	X
4	MG	F	1003	-	-	-	X
4	MG	G	1003	-	-	-	X
4	MG	H	1003	-	-	-	X

## 2 Entry composition

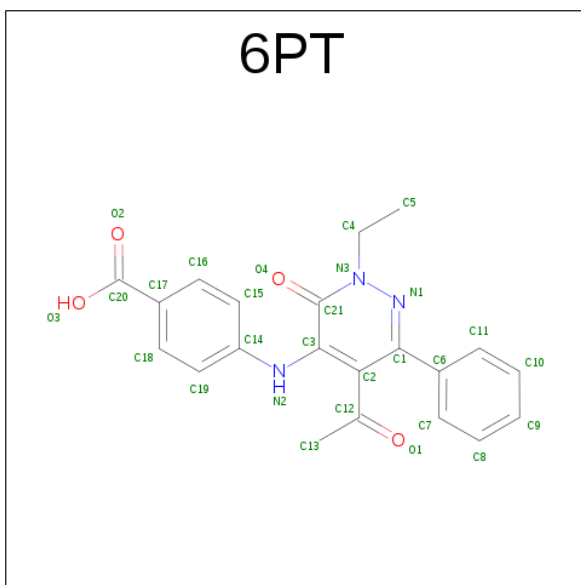
There are 5 unique types of molecules in this entry. The entry contains 21443 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2613	1655	446	498	14			
1	B	326	Total	C	N	O	S	0	0	0
			2637	1668	450	505	14			
1	C	321	Total	C	N	O	S	0	0	0
			2608	1652	445	497	14			
1	D	326	Total	C	N	O	S	0	0	0
			2638	1668	450	506	14			
1	E	321	Total	C	N	O	S	0	0	0
			2608	1652	445	497	14			
1	F	326	Total	C	N	O	S	0	0	0
			2638	1668	450	506	14			
1	G	322	Total	C	N	O	S	0	0	0
			2613	1655	446	498	14			
1	H	326	Total	C	N	O	S	0	0	0
			2638	1668	450	506	14			

- Molecule 2 is 4-[(5-acetyl-2-ethyl-3-oxo-6-phenyl-2,3-dihydropyridazin-4-yl)amino]benzoic acid (three-letter code: 6PT) (formula: C<sub>21</sub>H<sub>19</sub>N<sub>3</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	21	3	4		
2	B	1	Total	C	N	O	0	0
			28	21	3	4		
2	C	1	Total	C	N	O	0	0
			28	21	3	4		
2	D	1	Total	C	N	O	0	0
			28	21	3	4		
2	E	1	Total	C	N	O	0	0
			28	21	3	4		
2	F	1	Total	C	N	O	0	0
			28	21	3	4		
2	G	1	Total	C	N	O	0	0
			28	21	3	4		
2	H	1	Total	C	N	O	0	0
			28	21	3	4		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total 18	O 18	0	0
5	B	35	Total 35	O 35	0	0
5	C	33	Total 33	O 33	0	0
5	D	21	Total 21	O 21	0	0
5	E	32	Total 32	O 32	0	0

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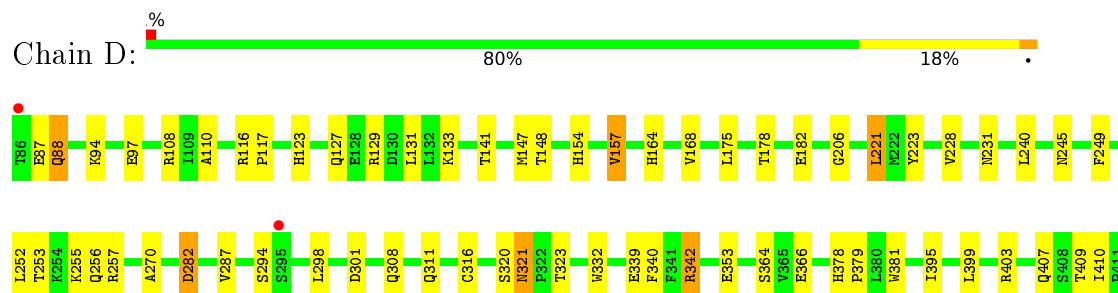
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	15	Total	O	0	0
			15	15		
5	G	33	Total	O	0	0
			33	33		
5	H	23	Total	O	0	0
			23	23		



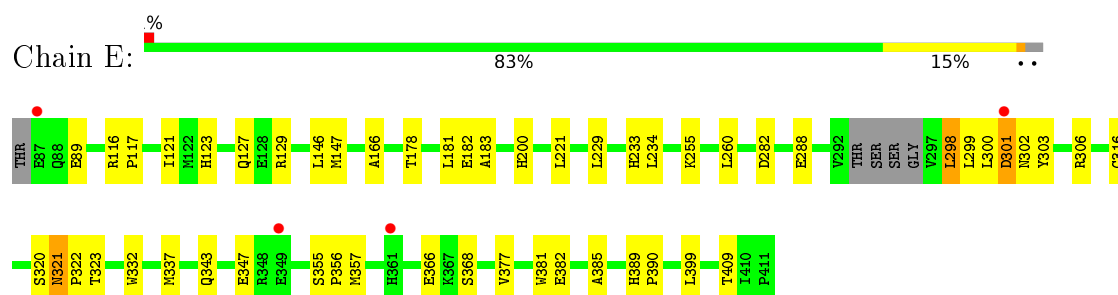


I410  
P411

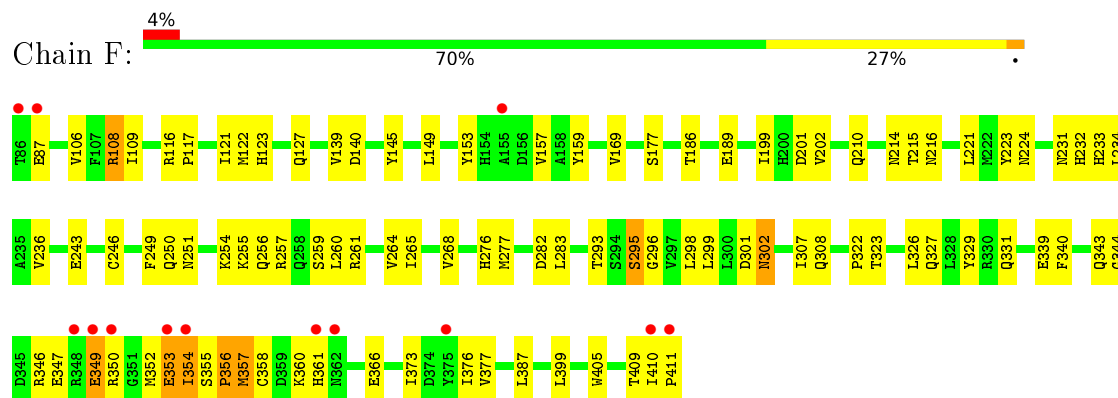
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



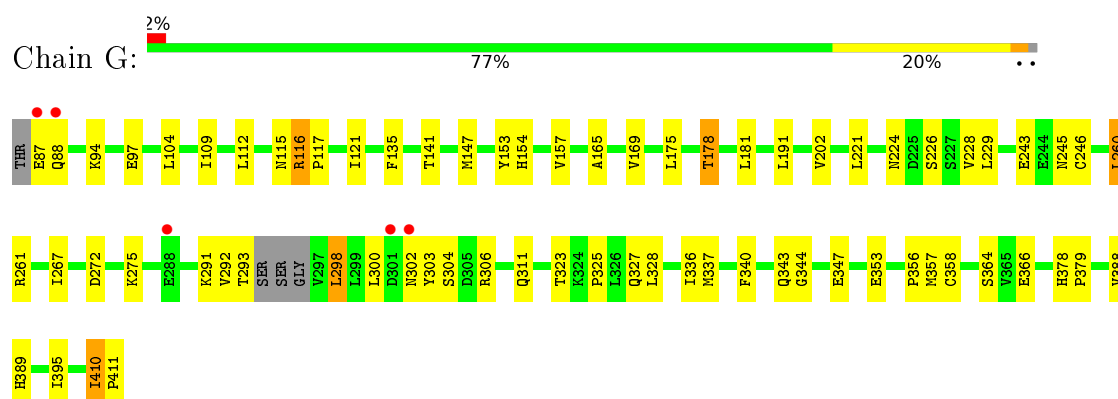
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



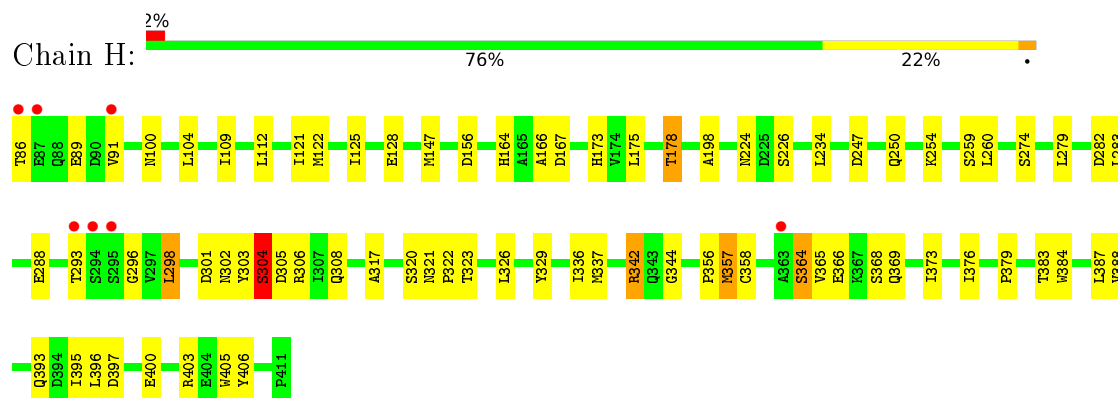
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



● Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.44Å 78.35Å 161.76Å 91.01° 92.79° 90.08°	Depositor
Resolution (Å)	25.00 – 2.61 24.98 – 2.61	Depositor EDS
% Data completeness (in resolution range)	94.8 (25.00-2.61) 94.5 (24.98-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.98 (at 2.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.191 , 0.258 0.197 , 0.261	Depositor DCC
$R_{free}$ test set	4408 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.077 for h,-k,-l 0.069 for -h,k,-l 0.065 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	21443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 6PT, ZN, MG

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	0.56	0/2666	0.66	0/3621
1	B	0.62	0/2691	0.71	0/3656
1	C	0.61	0/2661	0.72	0/3614
1	D	0.61	0/2692	0.71	1/3658 (0.0%)
1	E	0.64	0/2661	0.74	1/3614 (0.0%)
1	F	0.54	0/2692	0.65	0/3658
1	G	0.60	0/2666	0.69	0/3621
1	H	0.61	0/2692	0.70	0/3658
All	All	0.60	0/21421	0.70	2/29100 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	221	LEU	CA-CB-CG	-5.66	102.28	115.30
1	E	282	ASP	CB-CG-OD1	5.26	123.03	118.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2613	0	2565	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2637	0	2589	54	0
1	C	2608	0	2563	50	0
1	D	2638	0	2591	47	0
1	E	2608	0	2563	38	0
1	F	2638	0	2591	82	0
1	G	2613	0	2565	48	0
1	H	2638	0	2591	49	0
2	A	28	0	0	1	0
2	B	28	0	0	3	0
2	C	28	0	0	1	0
2	D	28	0	0	2	0
2	E	28	0	0	1	0
2	F	28	0	0	3	0
2	G	28	0	0	4	0
2	H	28	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	18	0	0	6	0
5	B	35	0	0	3	0
5	C	33	0	0	3	0
5	D	21	0	0	2	0
5	E	32	0	0	3	0
5	F	15	0	0	11	0
5	G	33	0	0	0	0
5	H	23	0	0	4	0
All	All	21443	0	20618	425	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (425) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:301:ASP:HB3	5:F:1109:HOH:O	1.18	1.27
1:C:411:PRO:HB3	5:C:1125:HOH:O	1.35	1.26
1:F:358:CYS:HB3	5:F:1103:HOH:O	1.02	1.17
1:F:331:GLN:HB3	5:F:1104:HOH:O	1.40	1.16
1:F:108:ARG:HH11	1:F:108:ARG:CG	1.57	1.14
1:H:337:MET:HE2	5:H:1106:HOH:O	1.45	1.13
1:A:357:MET:HE3	1:A:357:MET:HA	1.13	1.10
1:F:108:ARG:HH11	1:F:108:ARG:HG2	0.96	1.09
1:H:175:LEU:O	1:H:178:THR:HG22	1.49	1.09
1:E:337:MET:CE	5:E:1106:HOH:O	2.03	1.04
1:B:293:THR:HG23	1:B:299:LEU:HD21	1.37	1.04
1:A:358:CYS:HA	5:A:1107:HOH:O	1.60	1.01
1:H:86:THR:HB	1:H:89:GLU:OE1	1.61	1.00
1:B:357:MET:HE3	1:B:357:MET:HA	1.43	1.00
1:F:108:ARG:HG2	1:F:108:ARG:NH1	1.72	0.99
1:G:175:LEU:O	1:G:178:THR:HG22	1.69	0.93
1:D:342:ARG:CG	1:D:342:ARG:HH11	1.82	0.90
1:D:253:THR:OG1	1:D:256:GLN:HG3	1.70	0.90
1:D:342:ARG:HG2	1:D:342:ARG:HH11	1.37	0.89
1:E:306:ARG:HH11	1:E:306:ARG:HG2	1.35	0.89
1:D:407:GLN:HA	1:D:410:ILE:HD12	1.54	0.88
1:A:357:MET:HA	1:A:357:MET:CE	2.01	0.88
1:C:87:GLU:HG3	1:C:88:GLN:N	1.89	0.86
1:B:356:PRO:O	1:B:357:MET:HB2	1.74	0.85
1:F:123:HIS:CE1	1:F:127:GLN:HE21	1.92	0.85
1:H:337:MET:CE	5:H:1106:HOH:O	2.09	0.83
1:B:340:PHE:HZ	2:B:1001:6PT:C13	1.92	0.82
1:G:356:PRO:O	1:G:357:MET:HB2	1.80	0.80
1:B:193:ALA:HB2	1:B:310:LEU:HD22	1.63	0.79
1:B:357:MET:CE	1:B:357:MET:HA	2.11	0.79
1:F:373:ILE:HA	1:F:377:VAL:HB	1.65	0.79
1:E:306:ARG:NH1	1:E:306:ARG:HG2	1.98	0.77
1:H:125:ILE:HD13	1:H:173:HIS:HB2	1.67	0.76
1:C:324:LYS:NZ	5:C:1101:HOH:O	2.17	0.76
1:F:123:HIS:HE1	1:F:127:GLN:HE21	1.32	0.76
1:F:282:ASP:HB3	1:F:308:GLN:NE2	2.01	0.76
1:E:337:MET:HE1	5:E:1106:HOH:O	1.71	0.76
1:E:234:LEU:HB3	1:F:224:ASN:OD1	1.86	0.75
1:C:378:HIS:HB3	1:C:379:PRO:HD3	1.68	0.74
1:B:410:ILE:O	5:B:1101:HOH:O	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:PHE:HB3	5:A:1107:HOH:O	1.86	0.74
1:C:356:PRO:O	1:C:357:MET:HB2	1.86	0.74
1:F:356:PRO:O	1:F:357:MET:HB2	1.86	0.74
1:D:342:ARG:HG2	1:D:342:ARG:NH1	2.00	0.73
1:D:116:ARG:N	1:D:117:PRO:CD	2.51	0.73
1:H:393:GLN:NE2	1:H:397:ASP:OD1	2.21	0.73
1:B:86:THR:HB	1:B:89:GLU:OE1	1.88	0.72
1:B:175:LEU:O	1:B:178:THR:HG22	1.90	0.72
1:F:87:GLU:O	1:F:87:GLU:HG2	1.88	0.72
1:E:298:LEU:HD13	1:E:300:LEU:HD11	1.72	0.72
1:E:337:MET:HE3	5:E:1106:HOH:O	1.73	0.71
1:F:108:ARG:NH1	1:F:108:ARG:CG	2.29	0.71
1:G:104:LEU:HD11	1:G:109:ILE:HD11	1.74	0.70
1:D:94:LYS:O	1:D:97:GLU:HB2	1.93	0.69
1:A:357:MET:HE3	1:A:357:MET:CA	2.08	0.69
1:B:340:PHE:CZ	2:B:1001:6PT:C13	2.75	0.69
1:A:345:ASP:OD1	1:A:360:LYS:HE2	1.93	0.69
1:F:327:GLN:O	1:F:331:GLN:HG3	1.93	0.68
1:G:323:THR:HB	1:G:395:ILE:HG23	1.75	0.68
1:A:123:HIS:CE1	1:A:127:GLN:HE21	2.12	0.68
1:B:364:SER:OG	1:B:367:LYS:HB2	1.94	0.68
1:C:373:ILE:HG23	1:C:399:LEU:HD11	1.76	0.67
1:F:355:SER:HB2	1:F:358:CYS:SG	2.34	0.67
1:D:407:GLN:HA	1:D:410:ILE:CD1	2.25	0.67
1:C:132:LEU:CD2	1:C:139:VAL:HG23	2.24	0.66
1:G:366:GLU:N	1:G:366:GLU:OE2	2.25	0.66
1:G:298:LEU:HD13	1:G:300:LEU:HD21	1.77	0.65
1:D:116:ARG:CZ	1:D:147:MET:HE2	2.27	0.65
1:G:94:LYS:O	1:G:97:GLU:HB2	1.96	0.65
1:H:121:ILE:HD12	1:H:166:ALA:HB1	1.78	0.65
1:C:345:ASP:O	1:C:349:GLU:HG2	1.96	0.65
1:B:366:GLU:HG2	1:B:409:THR:OG1	1.97	0.65
1:G:154:HIS:HB2	1:G:157:VAL:HG13	1.77	0.64
1:B:293:THR:CG2	1:B:299:LEU:HD21	2.23	0.64
1:C:178:THR:HG22	1:C:181:LEU:HD12	1.80	0.64
1:F:327:GLN:HB3	5:F:1115:HOH:O	1.97	0.64
1:C:104:LEU:HD22	1:C:170:GLN:HG3	1.79	0.64
2:D:1001:6PT:C15	2:D:1001:6PT:C12	2.75	0.64
1:D:175:LEU:O	1:D:178:THR:HG22	1.98	0.64
1:G:243:GLU:O	1:G:246:CYS:HB2	1.98	0.63
1:A:136:LYS:O	1:A:251:ASN:ND2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:292:VAL:HG23	1:G:292:VAL:O	1.98	0.63
1:D:123:HIS:CE1	1:D:127:GLN:HE21	2.16	0.62
1:E:321:ASN:HB3	1:E:332:TRP:CD1	2.33	0.62
1:B:359:ASP:O	1:B:363:ALA:HB2	1.98	0.62
1:B:342:ARG:HH11	1:B:342:ARG:CG	2.13	0.62
1:C:286:MET:HE2	1:C:308:GLN:HB2	1.82	0.62
1:F:326:LEU:HD21	1:F:405:TRP:CD2	2.35	0.62
1:H:298:LEU:HD11	1:H:387:LEU:HD11	1.80	0.62
1:C:366:GLU:HG2	1:C:409:THR:OG1	1.99	0.62
1:B:123:HIS:CE1	1:B:127:GLN:HE21	2.19	0.61
1:F:302:ASN:ND2	1:F:302:ASN:H	1.98	0.61
1:G:141:THR:OG1	1:G:245:ASN:ND2	2.33	0.61
1:D:366:GLU:HG2	1:D:409:THR:OG1	2.01	0.61
1:H:282:ASP:HB3	1:H:308:GLN:NE2	2.16	0.61
2:H:1001:6PT:C15	2:H:1001:6PT:C12	2.78	0.61
1:B:104:LEU:HD22	1:B:170:GLN:HG3	1.83	0.61
1:F:340:PHE:HZ	2:F:1001:6PT:C13	2.14	0.61
1:B:345:ASP:OD1	1:B:360:LYS:HE2	2.00	0.60
1:C:356:PRO:O	1:C:357:MET:CB	2.47	0.60
1:F:327:GLN:CB	5:F:1115:HOH:O	2.50	0.60
1:A:301:ASP:HB3	5:A:1113:HOH:O	1.99	0.60
1:F:277:MET:HG2	5:F:1105:HOH:O	2.01	0.60
1:B:356:PRO:O	1:B:357:MET:CB	2.47	0.60
1:D:116:ARG:N	1:D:117:PRO:HD2	2.16	0.60
1:B:260:LEU:O	1:B:264:VAL:HG23	2.01	0.59
1:D:321:ASN:HB3	1:D:332:TRP:CD1	2.37	0.59
2:A:1001:6PT:C12	2:A:1001:6PT:C15	2.81	0.59
1:B:123:HIS:HE1	1:B:127:GLN:HE21	1.50	0.59
1:H:322:PRO:HB3	1:H:329:TYR:CZ	2.38	0.59
1:H:125:ILE:HD13	1:H:173:HIS:CB	2.32	0.59
1:H:303:TYR:O	1:H:305:ASP:N	2.35	0.59
1:F:366:GLU:HG2	1:F:409:THR:OG1	2.03	0.59
1:F:301:ASP:CB	5:F:1109:HOH:O	2.02	0.58
1:E:357:MET:SD	1:E:368:SER:OG	2.61	0.58
1:E:123:HIS:HE1	1:E:127:GLN:HE21	1.51	0.58
1:C:394:ASP:HB2	5:C:1117:HOH:O	2.02	0.58
1:A:404:GLU:O	1:A:404:GLU:HG3	2.04	0.58
2:C:1001:6PT:C15	2:C:1001:6PT:C12	2.82	0.58
1:E:260:LEU:C	1:E:260:LEU:HD23	2.23	0.58
1:E:356:PRO:O	1:E:357:MET:HB2	2.03	0.58
1:A:176:LEU:HD13	1:A:190:ILE:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:LEU:O	1:F:264:VAL:HG23	2.04	0.57
1:F:352:MET:O	1:F:354:ILE:N	2.37	0.57
1:C:304:SER:O	1:C:308:GLN:HG3	2.05	0.57
1:G:410:ILE:O	1:G:411:PRO:O	2.22	0.57
1:C:178:THR:CG2	1:C:181:LEU:HD12	2.35	0.57
1:H:356:PRO:O	1:H:357:MET:HB2	2.04	0.57
1:C:378:HIS:HB3	1:C:379:PRO:CD	2.35	0.57
1:F:243:GLU:O	1:F:246:CYS:HB2	2.05	0.56
1:F:356:PRO:O	1:F:357:MET:CB	2.53	0.56
1:A:239:LYS:HB2	1:B:221:LEU:HD21	1.86	0.56
1:G:302:ASN:OD1	1:G:304:SER:HB3	2.05	0.56
1:H:321:ASN:N	1:H:322:PRO:CD	2.68	0.56
1:D:154:HIS:HB2	1:D:157:VAL:HG13	1.88	0.56
1:C:210:GLN:HE21	1:C:214:ASN:ND2	2.04	0.56
1:A:344:GLY:HA2	1:A:347:GLU:HB2	1.87	0.56
1:C:87:GLU:CG	1:C:88:GLN:N	2.68	0.56
1:H:342:ARG:HD3	5:H:1115:HOH:O	2.06	0.56
1:A:393:GLN:HA	1:A:393:GLN:OE1	2.06	0.55
1:C:410:ILE:O	1:C:411:PRO:C	2.43	0.55
1:F:282:ASP:HB3	1:F:308:GLN:HE22	1.69	0.55
1:H:224:ASN:O	1:H:226:SER:HB2	2.06	0.55
1:D:141:THR:OG1	1:D:245:ASN:ND2	2.40	0.55
1:A:211:PHE:O	1:A:215:THR:HG23	2.07	0.55
1:A:285:THR:O	1:A:288:GLU:HB3	2.07	0.55
1:F:250:GLN:HA	1:F:257:ARG:HH12	1.71	0.55
1:B:94:LYS:O	1:B:97:GLU:HB2	2.07	0.55
1:F:87:GLU:O	1:F:87:GLU:CG	2.54	0.55
1:H:369:GLN:HG2	5:H:1106:HOH:O	2.06	0.55
1:D:182:GLU:OE2	1:D:182:GLU:HA	2.06	0.54
1:F:199:ILE:O	1:F:202:VAL:HG12	2.08	0.54
1:H:344:GLY:HA3	1:H:358:CYS:O	2.07	0.54
1:A:232:HIS:ND1	5:A:1101:HOH:O	2.30	0.54
1:D:228:VAL:HG23	5:D:1107:HOH:O	2.08	0.54
1:B:327:GLN:H	1:B:327:GLN:HE21	1.56	0.54
1:B:342:ARG:HH21	1:G:291:LYS:HE2	1.72	0.54
1:A:116:ARG:NH2	1:A:151:ASP:OD2	2.36	0.54
1:C:291:LYS:O	1:C:299:LEU:HB2	2.08	0.54
1:F:123:HIS:HE1	1:F:127:GLN:NE2	2.05	0.54
1:F:159:TYR:HB3	1:F:339:GLU:OE1	2.08	0.54
1:B:342:ARG:NH1	1:B:342:ARG:CG	2.70	0.54
1:A:154:HIS:HB2	1:A:157:VAL:HG13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:PHE:O	1:D:257:ARG:NH1	2.40	0.53
1:G:104:LEU:HD11	1:G:109:ILE:CD1	2.37	0.53
1:C:286:MET:CE	1:C:308:GLN:HB2	2.39	0.53
1:E:129:ARG:HH11	1:E:129:ARG:HG2	1.72	0.53
1:A:324:LYS:HB3	1:A:325:PRO:HD2	1.90	0.53
1:C:116:ARG:O	1:C:120:VAL:HG22	2.09	0.53
1:F:293:THR:O	1:F:296:GLY:N	2.35	0.53
1:A:92:LEU:O	1:A:96:LEU:HG	2.10	0.52
1:H:91:VAL:HG12	1:H:112:LEU:HD13	1.91	0.52
1:B:181:LEU:HD21	1:B:298:LEU:HD12	1.92	0.52
1:B:342:ARG:NH1	1:B:342:ARG:HG2	2.23	0.52
1:F:283:LEU:HD11	1:F:387:LEU:HD22	1.90	0.52
1:F:340:PHE:CZ	2:F:1001:6PT:C13	2.92	0.52
1:F:282:ASP:CB	1:F:308:GLN:NE2	2.70	0.52
1:F:254:LYS:O	1:F:255:LYS:C	2.47	0.52
1:A:340:PHE:CB	5:A:1107:HOH:O	2.52	0.52
1:D:116:ARG:NE	1:D:147:MET:HE2	2.23	0.52
1:E:343:GLN:O	1:E:347:GLU:HG3	2.09	0.52
1:G:116:ARG:NE	1:G:147:MET:HE2	2.25	0.52
1:G:292:VAL:CG2	1:G:292:VAL:O	2.57	0.52
1:E:116:ARG:CZ	1:E:147:MET:CE	2.88	0.52
1:B:321:ASN:HB2	1:B:332:TRP:CD1	2.45	0.51
1:D:323:THR:HB	1:D:395:ILE:HG23	1.91	0.51
1:G:340:PHE:HZ	2:G:1001:6PT:C13	2.23	0.51
1:G:154:HIS:HB2	1:G:157:VAL:CG1	2.38	0.51
1:D:164:HIS:O	1:D:168:VAL:HG23	2.11	0.51
1:H:317:ALA:HA	1:H:320:SER:HB3	1.92	0.51
1:F:326:LEU:HD21	1:F:405:TRP:CE3	2.46	0.51
1:C:321:ASN:N	1:C:322:PRO:CD	2.73	0.51
1:A:116:ARG:N	1:A:117:PRO:CD	2.73	0.50
1:C:299:LEU:O	1:C:300:LEU:HD23	2.11	0.50
1:E:322:PRO:HG2	1:E:377:VAL:HG21	1.94	0.50
1:F:123:HIS:O	1:F:127:GLN:HG2	2.12	0.50
1:H:326:LEU:HD21	1:H:405:TRP:CD2	2.47	0.50
1:A:357:MET:SD	1:A:368:SER:OG	2.54	0.50
1:B:184:VAL:HG11	1:B:300:LEU:HD12	1.91	0.50
1:B:321:ASN:CB	1:B:332:TRP:CD1	2.95	0.50
1:F:108:ARG:HH11	1:F:108:ARG:HG3	1.63	0.50
1:F:355:SER:HB3	1:F:356:PRO:CD	2.42	0.50
1:G:135:PHE:CE2	1:G:191:LEU:HD22	2.47	0.50
1:C:253:THR:HB	1:E:288:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:369:GLN:O	1:H:373:ILE:HG13	2.11	0.49
1:A:200:HIS:NE2	1:A:201:ASP:OD2	2.45	0.49
1:A:340:PHE:C	5:A:1107:HOH:O	2.49	0.49
1:F:302:ASN:HD22	1:F:302:ASN:H	1.58	0.49
1:A:366:GLU:HG2	1:A:409:THR:OG1	2.12	0.49
1:D:301:ASP:N	5:D:1102:HOH:O	2.30	0.49
1:G:336:ILE:HG23	1:G:337:MET:HE2	1.94	0.49
1:E:123:HIS:CE1	1:E:127:GLN:HE21	2.29	0.49
1:F:357:MET:CE	1:F:357:MET:HA	2.42	0.49
1:C:132:LEU:HD22	1:C:139:VAL:HG23	1.95	0.49
1:C:323:THR:HB	1:C:395:ILE:HG23	1.94	0.49
1:D:282:ASP:HB3	1:D:308:GLN:NE2	2.28	0.49
1:G:302:ASN:O	1:G:306:ARG:HG3	2.12	0.49
1:E:116:ARG:CZ	1:E:147:MET:HE3	2.42	0.49
1:B:243:GLU:O	1:B:244:GLU:C	2.49	0.49
2:E:1001:6PT:C12	2:E:1001:6PT:C15	2.91	0.49
1:E:366:GLU:HG2	1:E:409:THR:OG1	2.12	0.48
1:C:373:ILE:CG2	1:C:399:LEU:HD11	2.43	0.48
1:F:122:MET:SD	1:F:169:VAL:HG11	2.53	0.48
2:G:1001:6PT:C15	2:G:1001:6PT:C12	2.91	0.48
1:G:224:ASN:OD1	1:H:234:LEU:HB3	2.12	0.48
1:D:123:HIS:HE1	1:D:127:GLN:HE21	1.60	0.48
1:D:342:ARG:HH11	1:D:342:ARG:HG3	1.74	0.48
1:B:327:GLN:NE2	1:B:327:GLN:H	2.10	0.48
1:C:337:MET:HG3	1:C:365:VAL:HG22	1.95	0.48
1:D:116:ARG:CZ	1:D:147:MET:CE	2.91	0.48
1:H:337:MET:HE3	1:H:365:VAL:HA	1.96	0.48
1:A:355:SER:HB3	1:A:356:PRO:CD	2.43	0.48
1:B:323:THR:HG22	1:B:399:LEU:HD13	1.95	0.48
1:E:301:ASP:O	1:E:302:ASN:HB3	2.13	0.48
1:F:344:GLY:HA2	1:F:347:GLU:HB2	1.95	0.48
1:D:342:ARG:CG	1:D:342:ARG:NH1	2.53	0.48
1:H:125:ILE:HD13	1:H:173:HIS:CG	2.49	0.48
1:E:116:ARG:N	1:E:117:PRO:CD	2.77	0.47
1:F:106:VAL:HA	1:F:109:ILE:HD12	1.95	0.47
1:F:344:GLY:CA	5:F:1103:HOH:O	2.62	0.47
2:F:1001:6PT:C15	2:F:1001:6PT:C12	2.92	0.47
1:F:410:ILE:CG2	1:F:411:PRO:HD2	2.44	0.47
1:H:100:ASN:OD1	1:H:173:HIS:NE2	2.43	0.47
1:A:315:HIS:CE1	1:A:319:LEU:HD11	2.50	0.47
1:D:316:CYS:HB3	1:D:381:TRP:CZ2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:ASN:O	1:E:303:TYR:C	2.52	0.47
2:B:1001:6PT:C12	2:B:1001:6PT:C15	2.93	0.47
1:D:253:THR:HG1	1:D:256:GLN:HG3	1.78	0.47
1:F:293:THR:C	1:F:295:SER:N	2.68	0.47
1:D:110:ALA:HA	1:D:117:PRO:HD3	1.95	0.47
1:F:234:LEU:HD21	1:F:268:VAL:HB	1.96	0.47
1:F:344:GLY:N	5:F:1103:HOH:O	2.48	0.47
1:G:410:ILE:HG22	1:G:411:PRO:N	2.30	0.47
1:F:215:THR:O	1:F:216:ASN:C	2.53	0.46
1:C:178:THR:OG1	1:C:391:ASP:OD2	2.31	0.46
1:D:148:THR:HG22	1:D:240:LEU:HD22	1.97	0.46
1:B:121:ILE:HD12	1:B:166:ALA:HB1	1.97	0.46
1:D:129:ARG:HB2	1:D:131:LEU:HG	1.98	0.46
1:G:117:PRO:O	1:G:121:ILE:HD12	2.15	0.46
1:E:182:GLU:O	1:E:183:ALA:HB3	2.16	0.46
1:E:298:LEU:HD13	1:E:300:LEU:CD1	2.43	0.46
1:F:254:LYS:C	1:F:256:GLN:N	2.68	0.46
1:H:323:THR:HB	1:H:395:ILE:HG23	1.97	0.46
1:G:178:THR:CG2	1:G:181:LEU:HD12	2.45	0.46
1:H:279:LEU:HD12	1:H:279:LEU:HA	1.77	0.46
1:A:348:ARG:HB3	1:A:348:ARG:HH11	1.79	0.46
1:F:157:VAL:O	1:F:157:VAL:HG23	2.16	0.46
1:G:292:VAL:O	1:G:293:THR:C	2.52	0.46
1:H:384:TRP:O	1:H:388:VAL:HG22	2.15	0.46
1:D:407:GLN:CA	1:D:410:ILE:HD12	2.36	0.46
1:E:129:ARG:HG2	1:E:129:ARG:NH1	2.31	0.46
1:G:340:PHE:CZ	2:G:1001:6PT:C13	2.98	0.46
1:F:210:GLN:HE21	1:F:214:ASN:ND2	2.13	0.46
1:A:345:ASP:HA	1:A:348:ARG:HH12	1.81	0.46
1:A:178:THR:OG1	1:A:391:ASP:CB	2.64	0.46
1:F:349:GLU:O	1:F:350:ARG:C	2.54	0.46
1:H:322:PRO:HA	1:H:329:TYR:CD1	2.51	0.46
1:A:316:CYS:O	1:A:320:SER:HB3	2.16	0.45
1:B:230:GLU:OE2	1:B:272:ASP:HA	2.16	0.45
1:B:331:GLN:HB3	5:B:1122:HOH:O	2.16	0.45
1:C:210:GLN:HE21	1:C:214:ASN:HD21	1.63	0.45
1:A:367:LYS:HB2	1:A:367:LYS:HE3	1.65	0.45
1:H:298:LEU:HD11	1:H:387:LEU:CD1	2.44	0.45
1:F:358:CYS:CB	5:F:1103:HOH:O	1.90	0.45
1:H:364:SER:O	1:H:368:SER:OG	2.28	0.45
1:A:224:ASN:OD1	1:B:234:LEU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:CYS:O	1:E:320:SER:HB3	2.17	0.45
1:F:116:ARG:N	1:F:117:PRO:CD	2.80	0.45
1:A:270:ALA:HB1	1:A:279:LEU:HD21	1.97	0.45
1:A:299:LEU:O	1:A:300:LEU:HD23	2.17	0.45
1:C:301:ASP:O	1:C:302:ASN:CB	2.64	0.45
1:E:121:ILE:HD12	1:E:166:ALA:HB1	1.99	0.45
1:C:367:LYS:HB2	1:C:367:LYS:HE3	1.68	0.45
1:H:303:TYR:O	1:H:304:SER:C	2.55	0.45
1:C:301:ASP:O	1:C:302:ASN:HB3	2.17	0.45
1:C:364:SER:HB3	1:C:367:LYS:HB3	1.98	0.45
1:F:323:THR:HG22	1:F:399:LEU:HD13	1.99	0.45
1:B:342:ARG:NH2	1:G:291:LYS:HE2	2.31	0.45
1:G:410:ILE:HB	1:G:411:PRO:HD3	1.98	0.45
1:H:104:LEU:HD11	1:H:109:ILE:CD1	2.47	0.45
1:H:254:LYS:HB2	1:H:254:LYS:HE3	1.64	0.45
1:D:316:CYS:O	1:D:320:SER:HB3	2.17	0.45
1:F:186:THR:N	1:F:189:GLU:OE1	2.42	0.45
1:G:298:LEU:CD1	1:G:300:LEU:HD21	2.45	0.45
1:C:288:GLU:OE2	1:C:288:GLU:HA	2.16	0.45
1:F:108:ARG:NH1	1:F:108:ARG:HG3	2.27	0.45
1:F:250:GLN:HG3	1:F:251:ASN:OD1	2.17	0.45
1:G:302:ASN:O	1:G:303:TYR:C	2.56	0.45
1:H:156:ASP:N	1:H:156:ASP:OD2	2.51	0.44
1:D:206:GLY:HA2	1:D:339:GLU:OE2	2.17	0.44
1:H:247:ASP:O	1:H:250:GLN:HG2	2.17	0.44
1:C:303:TYR:HA	1:C:306:ARG:HD3	1.98	0.44
1:D:223:TYR:CE1	1:D:231:ASN:HB3	2.52	0.44
1:D:87:GLU:O	1:D:88:GLN:C	2.55	0.44
1:C:234:LEU:HD11	1:C:268:VAL:HB	1.99	0.44
1:D:116:ARG:NE	1:D:147:MET:CE	2.80	0.44
1:B:329:TYR:CE2	1:B:406:TYR:HE2	2.35	0.44
1:A:191:LEU:HD23	1:A:260:LEU:HD13	1.99	0.44
1:E:381:TRP:O	1:E:385:ALA:N	2.48	0.44
1:F:117:PRO:O	1:F:121:ILE:HG13	2.17	0.44
1:G:260:LEU:O	1:G:261:ARG:C	2.56	0.44
1:E:229:LEU:HA	1:E:229:LEU:HD23	1.88	0.44
1:E:323:THR:HG22	1:E:399:LEU:HD13	2.00	0.44
1:E:321:ASN:CB	1:E:332:TRP:CD1	3.01	0.44
1:A:355:SER:HB2	1:A:358:CYS:HB2	2.00	0.43
1:D:270:ALA:CB	1:D:311:GLN:HG2	2.47	0.43
1:E:306:ARG:CG	1:E:306:ARG:HH11	2.13	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:LYS:HG3	1:F:361:HIS:CD2	2.53	0.43
1:B:307:ILE:CG2	1:B:308:GLN:N	2.81	0.43
1:G:88:GLN:OE1	1:G:112:LEU:O	2.36	0.43
1:H:104:LEU:HD11	1:H:109:ILE:HD11	2.00	0.43
1:B:181:LEU:CD2	1:B:298:LEU:HD12	2.49	0.43
1:H:283:LEU:HG	1:H:383:THR:HG22	1.99	0.43
1:B:302:ASN:OD1	1:B:304:SER:HB3	2.18	0.43
1:C:286:MET:HE2	1:C:308:GLN:CB	2.47	0.43
1:E:200:HIS:O	1:E:233:HIS:CD2	2.72	0.43
1:F:223:TYR:CE1	1:F:231:ASN:HB3	2.54	0.43
1:A:207:VAL:HG11	1:A:346:ARG:NH1	2.33	0.43
1:B:139:VAL:HG13	1:B:140:ASP:N	2.34	0.43
1:B:154:HIS:HB2	1:B:157:VAL:HG13	2.00	0.43
1:D:340:PHE:CZ	2:D:1001:6PT:C13	3.02	0.43
1:F:276:HIS:CD2	1:F:376:ILE:HD12	2.54	0.43
1:A:201:ASP:HA	1:A:233:HIS:CD2	2.54	0.43
1:D:378:HIS:O	1:D:379:PRO:C	2.54	0.43
1:D:88:GLN:HB2	1:D:88:GLN:HE21	1.67	0.43
1:F:322:PRO:HA	1:F:329:TYR:CG	2.54	0.43
1:A:348:ARG:HG3	1:A:354:ILE:HD11	2.01	0.43
1:A:88:GLN:O	1:A:88:GLN:HG2	2.19	0.43
1:G:154:HIS:CB	1:G:157:VAL:HG13	2.46	0.42
1:G:344:GLY:HA3	1:G:358:CYS:O	2.19	0.42
1:H:125:ILE:O	1:H:128:GLU:HB3	2.19	0.42
1:A:389:HIS:HA	1:A:390:PRO:HA	1.68	0.42
1:B:286:MET:HE3	1:B:286:MET:HB2	1.87	0.42
1:C:121:ILE:O	1:C:125:ILE:HD12	2.19	0.42
1:C:168:VAL:HG21	1:C:200:HIS:CE1	2.54	0.42
1:F:322:PRO:HA	1:F:329:TYR:CD1	2.54	0.42
1:G:267:ILE:HA	1:G:311:GLN:HG2	2.00	0.42
1:B:329:TYR:CE2	1:B:406:TYR:CE2	3.07	0.42
1:C:192:ALA:HB2	1:C:263:MET:HE3	2.02	0.42
1:D:154:HIS:CB	1:D:157:VAL:HG13	2.48	0.42
1:C:253:THR:OG1	1:C:256:GLN:HG3	2.19	0.42
1:H:302:ASN:ND2	1:H:302:ASN:H	2.17	0.42
1:H:122:MET:CE	1:H:198:ALA:HB2	2.49	0.42
1:A:200:HIS:O	1:A:233:HIS:CD2	2.73	0.42
1:B:116:ARG:N	1:B:117:PRO:CD	2.83	0.42
1:E:316:CYS:HB3	1:E:381:TRP:CZ2	2.54	0.42
1:G:272:ASP:HB3	1:G:275:LYS:HD2	2.01	0.42
1:H:326:LEU:HD12	1:H:326:LEU:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:GLN:O	1:C:331:GLN:HG3	2.18	0.42
1:E:146:LEU:HD23	1:E:146:LEU:HA	1.80	0.42
1:E:389:HIS:HA	1:E:390:PRO:HA	1.76	0.42
1:G:165:ALA:O	1:G:169:VAL:HG23	2.20	0.42
1:G:229:LEU:HA	1:G:229:LEU:HD23	1.81	0.42
1:C:127:GLN:HA	1:C:127:GLN:OE1	2.20	0.42
1:G:175:LEU:HD23	1:G:175:LEU:HA	1.91	0.42
1:B:253:THR:HB	5:B:1114:HOH:O	2.20	0.42
1:G:115:ASN:C	1:G:117:PRO:HD2	2.40	0.42
1:G:325:PRO:HD2	1:G:328:LEU:HD12	2.02	0.42
1:A:215:THR:O	1:A:216:ASN:C	2.58	0.41
1:B:307:ILE:HA	1:B:307:ILE:HD12	1.79	0.41
1:F:153:TYR:CE2	1:F:202:VAL:HA	2.55	0.41
1:A:357:MET:HE1	1:A:364:SER:H	1.85	0.41
1:A:378:HIS:HB3	1:A:379:PRO:HD3	2.02	0.41
1:A:178:THR:OG1	1:A:391:ASP:HB3	2.20	0.41
1:B:176:LEU:HD13	1:B:190:ILE:HG23	2.03	0.41
1:A:201:ASP:HA	1:A:233:HIS:CG	2.56	0.41
1:A:243:GLU:HB2	1:A:246:CYS:SG	2.61	0.41
1:A:346:ARG:HA	1:A:349:GLU:HB2	2.02	0.41
1:G:153:TYR:CE2	1:G:202:VAL:HA	2.55	0.41
1:G:378:HIS:HB3	1:G:379:PRO:HD3	2.02	0.41
1:H:329:TYR:CE2	1:H:406:TYR:HE2	2.38	0.41
1:A:253:THR:OG1	1:A:256:GLN:HB2	2.21	0.41
1:B:302:ASN:O	1:B:306:ARG:HG3	2.21	0.41
1:C:404:GLU:OE1	1:C:404:GLU:HA	2.21	0.41
1:C:410:ILE:HB	1:C:411:PRO:CD	2.50	0.41
1:D:321:ASN:CB	1:D:332:TRP:CD1	3.04	0.41
1:F:232:HIS:O	1:F:236:VAL:HG23	2.21	0.41
1:F:327:GLN:HB2	5:F:1115:HOH:O	2.18	0.41
1:H:366:GLU:H	1:H:366:GLU:CD	2.24	0.41
1:B:337:MET:HG3	1:B:365:VAL:HG22	2.03	0.41
1:D:323:THR:HG22	1:D:399:LEU:HB2	2.02	0.41
1:F:201:ASP:HA	1:F:233:HIS:CD2	2.55	0.41
1:G:337:MET:HE1	2:G:1001:6PT:C8	2.51	0.41
1:A:410:ILE:HG22	1:A:411:PRO:N	2.35	0.41
1:C:229:LEU:HB3	1:C:233:HIS:NE2	2.36	0.41
1:H:164:HIS:O	1:H:167:ASP:HB3	2.21	0.41
1:A:201:ASP:HA	1:A:233:HIS:CE1	2.55	0.41
1:A:226:SER:O	1:A:227:SER:C	2.59	0.41
1:G:343:GLN:O	1:G:347:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:396:LEU:HA	1:H:396:LEU:HD12	1.92	0.41
1:E:178:THR:HG22	1:E:181:LEU:HD12	2.03	0.41
1:H:376:ILE:C	1:H:379:PRO:HD2	2.41	0.41
1:F:353:GLU:O	1:F:354:ILE:C	2.59	0.40
1:G:388:VAL:O	1:G:389:HIS:C	2.59	0.40
1:H:396:LEU:O	1:H:400:GLU:HG3	2.21	0.40
1:C:170:GLN:O	1:C:173:HIS:HB3	2.22	0.40
1:F:302:ASN:N	1:F:302:ASN:ND2	2.66	0.40
1:F:355:SER:HB3	1:F:356:PRO:HD3	2.04	0.40
1:D:252:LEU:HB3	1:D:256:GLN:HB2	2.03	0.40
1:F:145:TYR:CE2	1:F:149:LEU:HD22	2.56	0.40
1:B:132:LEU:HD12	1:B:132:LEU:H	1.87	0.40
1:F:249:PHE:O	1:F:257:ARG:NH1	2.54	0.40
1:F:139:VAL:HG13	1:F:140:ASP:N	2.37	0.40
1:F:261:ARG:O	1:F:265:ILE:HG13	2.21	0.40
1:F:343:GLN:O	1:F:346:ARG:HB2	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	318/326 (98%)	286 (90%)	29 (9%)	3 (1%)	21	41
1	B	324/326 (99%)	306 (94%)	17 (5%)	1 (0%)	46	70
1	C	317/326 (97%)	299 (94%)	18 (6%)	0	100	100
1	D	324/326 (99%)	306 (94%)	18 (6%)	0	100	100
1	E	317/326 (97%)	301 (95%)	16 (5%)	0	100	100
1	F	324/326 (99%)	284 (88%)	35 (11%)	5 (2%)	13	24
1	G	318/326 (98%)	293 (92%)	22 (7%)	3 (1%)	21	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	324/326 (99%)	301 (93%)	20 (6%)	3 (1%)	21	41
All	All	2566/2608 (98%)	2376 (93%)	175 (7%)	15 (1%)	30	54

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	353	GLU
1	F	357	MET
1	G	410	ILE
1	H	304	SER
1	F	349	GLU
1	H	301	ASP
1	A	112	LEU
1	B	290	LYS
1	F	356	PRO
1	H	296	GLY
1	A	355	SER
1	A	410	ILE
1	G	228	VAL
1	F	354	ILE
1	G	116	ARG

### 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	294/298 (99%)	280 (95%)	14 (5%)	31	57
1	B	297/298 (100%)	287 (97%)	10 (3%)	44	71
1	C	294/298 (99%)	284 (97%)	10 (3%)	44	71
1	D	298/298 (100%)	283 (95%)	15 (5%)	30	55
1	E	294/298 (99%)	285 (97%)	9 (3%)	47	75
1	F	298/298 (100%)	289 (97%)	9 (3%)	48	75
1	G	294/298 (99%)	285 (97%)	9 (3%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	298/298 (100%)	283 (95%)	15 (5%)	30	55
All	All	2367/2384 (99%)	2276 (96%)	91 (4%)	40	68

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLU
1	A	108	ARG
1	A	219	LEU
1	A	221	LEU
1	A	244	GLU
1	A	245	ASN
1	A	255	LYS
1	A	260	LEU
1	A	279	LEU
1	A	298	LEU
1	A	327	GLN
1	A	357	MET
1	A	364	SER
1	A	404	GLU
1	B	108	ARG
1	B	133	LYS
1	B	148	THR
1	B	245	ASN
1	B	259	SER
1	B	293	THR
1	B	295	SER
1	B	327	GLN
1	B	342	ARG
1	B	357	MET
1	C	87	GLU
1	C	99	VAL
1	C	139	VAL
1	C	226	SER
1	C	254	LYS
1	C	259	SER
1	C	298	LEU
1	C	299	LEU
1	C	304	SER
1	C	362	ASN
1	D	88	GLN
1	D	108	ARG

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Mol	Chain	Res	Type
1	D	133	LYS
1	D	157	VAL
1	D	221	LEU
1	D	255	LYS
1	D	282	ASP
1	D	287	VAL
1	D	294	SER
1	D	298	LEU
1	D	321	ASN
1	D	342	ARG
1	D	353	GLU
1	D	364	SER
1	D	403	ARG
1	E	89	GLU
1	E	221	LEU
1	E	255	LYS
1	E	298	LEU
1	E	299	LEU
1	E	301	ASP
1	E	321	ASN
1	E	355	SER
1	E	382	GLU
1	F	108	ARG
1	F	177	SER
1	F	221	LEU
1	F	259	SER
1	F	295	SER
1	F	298	LEU
1	F	299	LEU
1	F	302	ASN
1	F	307	ILE
1	G	87	GLU
1	G	178	THR
1	G	221	LEU
1	G	226	SER
1	G	260	LEU
1	G	298	LEU
1	G	327	GLN
1	G	353	GLU
1	G	364	SER
1	H	147	MET
1	H	178	THR

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Mol	Chain	Res	Type
1	H	259	SER
1	H	260	LEU
1	H	274	SER
1	H	288	GLU
1	H	293	THR
1	H	298	LEU
1	H	304	SER
1	H	306	ARG
1	H	336	ILE
1	H	342	ARG
1	H	357	MET
1	H	364	SER
1	H	403	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	123	HIS
1	A	245	ASN
1	B	88	GLN
1	B	123	HIS
1	B	210	GLN
1	B	245	ASN
1	B	308	GLN
1	B	327	GLN
1	C	88	GLN
1	C	210	GLN
1	C	242	GLN
1	C	245	ASN
1	C	258	GLN
1	D	88	GLN
1	D	123	HIS
1	D	242	GLN
1	D	245	ASN
1	D	321	ASN
1	D	389	HIS
1	E	123	HIS
1	E	210	GLN
1	E	242	GLN
1	E	245	ASN
1	E	250	GLN

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Mol	Chain	Res	Type
1	E	308	GLN
1	E	321	ASN
1	E	369	GLN
1	F	88	GLN
1	F	123	HIS
1	F	210	GLN
1	F	245	ASN
1	F	302	ASN
1	F	308	GLN
1	F	362	ASN
1	F	369	GLN
1	G	88	GLN
1	G	123	HIS
1	G	245	ASN
1	G	258	GLN
1	H	88	GLN
1	H	210	GLN
1	H	242	GLN
1	H	245	ASN
1	H	302	ASN
1	H	308	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	6PT	A	1001	-	24,30,30	0.77	1 (4%)	25,42,42	1.33	3 (12%)
2	6PT	B	1001	-	24,30,30	0.85	2 (8%)	25,42,42	1.41	2 (8%)
2	6PT	C	1001	-	24,30,30	0.67	0	25,42,42	1.44	4 (16%)
2	6PT	D	1001	-	24,30,30	0.65	1 (4%)	25,42,42	1.60	7 (28%)
2	6PT	E	1001	-	24,30,30	0.94	1 (4%)	25,42,42	1.69	7 (28%)
2	6PT	F	1001	-	24,30,30	0.63	0	25,42,42	1.57	4 (16%)
2	6PT	G	1001	-	24,30,30	0.82	1 (4%)	25,42,42	1.56	5 (20%)
2	6PT	H	1001	-	24,30,30	0.89	1 (4%)	25,42,42	1.88	6 (24%)

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	6PT	A	1001	-	-	0/13/18/18	0/3/3/3
2	6PT	B	1001	-	-	0/13/18/18	0/3/3/3
2	6PT	C	1001	-	-	0/13/18/18	0/3/3/3
2	6PT	D	1001	-	-	0/13/18/18	0/3/3/3
2	6PT	E	1001	-	-	0/13/18/18	0/3/3/3
2	6PT	F	1001	-	-	0/13/18/18	0/3/3/3
2	6PT	G	1001	-	-	0/13/18/18	0/3/3/3
2	6PT	H	1001	-	-	0/13/18/18	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1001	6PT	C21-C3	-3.05	1.37	1.41
2	B	1001	6PT	C21-C3	-2.05	1.38	1.41
2	D	1001	6PT	C1-N1	2.02	1.35	1.33
2	B	1001	6PT	C1-N1	2.12	1.35	1.33
2	E	1001	6PT	C1-N1	2.87	1.36	1.33
2	A	1001	6PT	C1-N1	2.88	1.36	1.33
2	H	1001	6PT	C1-N1	3.18	1.36	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1001	6PT	C7-C6-C1	-4.43	113.69	120.60
2	H	1001	6PT	C2-C1-C6	-3.90	118.07	123.51
2	F	1001	6PT	C7-C6-C1	-3.83	114.63	120.60
2	D	1001	6PT	O1-C12-C2	-3.44	113.29	119.97
2	F	1001	6PT	O1-C12-C2	-3.39	113.39	119.97
2	A	1001	6PT	C7-C6-C1	-3.29	115.47	120.60
2	E	1001	6PT	C16-C17-C20	-3.07	116.38	120.43
2	G	1001	6PT	C15-C16-C17	-2.97	116.97	121.15
2	G	1001	6PT	C7-C6-C1	-2.83	116.19	120.60
2	C	1001	6PT	C7-C6-C1	-2.59	116.56	120.60
2	D	1001	6PT	C7-C6-C1	-2.58	116.58	120.60
2	E	1001	6PT	O1-C12-C2	-2.38	115.34	119.97
2	G	1001	6PT	C18-C19-C14	-2.38	117.62	120.30
2	B	1001	6PT	O1-C12-C2	-2.18	115.74	119.97
2	G	1001	6PT	C15-C14-N2	-2.17	113.48	120.66
2	H	1001	6PT	O1-C12-C2	-2.15	115.80	119.97
2	F	1001	6PT	C10-C11-C6	-2.07	117.84	120.56
2	D	1001	6PT	C16-C17-C20	-2.07	117.71	120.43
2	C	1001	6PT	C2-C1-C6	-2.06	120.64	123.51
2	E	1001	6PT	C18-C17-C20	2.03	123.09	120.43
2	E	1001	6PT	C11-C6-C1	2.06	123.80	120.60
2	D	1001	6PT	C11-C6-C1	2.08	123.83	120.60
2	D	1001	6PT	C6-C1-N1	2.09	116.74	114.38
2	A	1001	6PT	C6-C1-N1	2.23	116.90	114.38
2	D	1001	6PT	C18-C17-C20	2.24	123.38	120.43
2	C	1001	6PT	C6-C1-N1	2.24	116.91	114.38
2	E	1001	6PT	C3-N2-C14	2.29	133.19	124.99
2	C	1001	6PT	C13-C12-C2	2.40	127.42	120.27
2	H	1001	6PT	C13-C12-C2	2.47	127.63	120.27
2	E	1001	6PT	C13-C12-C2	2.49	127.69	120.27
2	F	1001	6PT	C11-C6-C1	2.51	124.51	120.60
2	D	1001	6PT	C13-C12-C2	2.58	127.96	120.27
2	A	1001	6PT	C11-C6-C1	2.60	124.65	120.60
2	H	1001	6PT	C11-C6-C1	3.06	125.37	120.60
2	G	1001	6PT	C16-C15-C14	3.21	123.90	120.30
2	B	1001	6PT	C6-C1-N1	3.35	118.17	114.38
2	H	1001	6PT	C6-C1-N1	3.75	118.61	114.38
2	E	1001	6PT	C6-C1-N1	3.80	118.67	114.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	6PT	1	0
2	B	1001	6PT	3	0
2	C	1001	6PT	1	0
2	D	1001	6PT	2	0
2	E	1001	6PT	1	0
2	F	1001	6PT	3	0
2	G	1001	6PT	4	0
2	H	1001	6PT	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	322/326 (98%)	-0.12	6 (1%) 70 65	22, 36, 59, 82	0
1	B	326/326 (100%)	-0.31	2 (0%) 90 88	15, 27, 48, 63	0
1	C	321/326 (98%)	-0.27	3 (0%) 85 83	17, 26, 44, 55	0
1	D	326/326 (100%)	-0.35	2 (0%) 90 88	17, 26, 45, 65	0
1	E	321/326 (98%)	-0.33	4 (1%) 81 77	14, 24, 42, 52	0
1	F	326/326 (100%)	-0.04	13 (3%) 42 35	22, 37, 63, 83	0
1	G	322/326 (98%)	-0.36	5 (1%) 74 69	16, 27, 43, 63	0
1	H	326/326 (100%)	-0.16	7 (2%) 67 61	17, 30, 50, 71	0
All	All	2590/2608 (99%)	-0.24	42 (1%) 74 69	14, 29, 52, 83	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	411	PRO	5.2
1	H	86	THR	4.9
1	H	295	SER	4.3
1	F	353	GLU	4.0
1	F	86	THR	3.5
1	C	411	PRO	3.4
1	E	87	GLU	3.3
1	A	356	PRO	3.3
1	F	410	ILE	3.2
1	F	361	HIS	3.2
1	F	87	GLU	3.1
1	A	353	GLU	2.9
1	H	294	SER	2.8
1	C	362	ASN	2.7
1	G	301	ASP	2.7
1	H	363	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	87	GLU	2.6
1	B	295	SER	2.6
1	F	362	ASN	2.5
1	F	354	ILE	2.5
1	H	87	GLU	2.5
1	E	301	ASP	2.4
1	D	295	SER	2.4
1	G	288	GLU	2.4
1	F	348	ARG	2.4
1	F	155	ALA	2.4
1	B	87	GLU	2.3
1	A	105	HIS	2.2
1	A	90	ASP	2.2
1	D	86	THR	2.2
1	G	87	GLU	2.2
1	A	349	GLU	2.1
1	G	88	GLN	2.1
1	G	302	ASN	2.1
1	E	361	HIS	2.1
1	F	375	TYR	2.1
1	A	292	VAL	2.1
1	F	349	GLU	2.1
1	E	349	GLU	2.1
1	H	293	THR	2.0
1	F	350	ARG	2.0
1	H	91	VAL	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 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
4	MG	H	1003	1/1	0.87	0.62	55.18	38,38,38,38	0
4	MG	B	1003	1/1	0.94	0.64	46.70	37,37,37,37	0
4	MG	F	1003	1/1	0.96	0.55	27.80	37,37,37,37	0
4	MG	D	1003	1/1	0.95	0.63	26.80	34,34,34,34	0
4	MG	C	1003	1/1	0.95	0.59	23.77	38,38,38,38	0
4	MG	G	1003	1/1	0.94	0.67	21.32	35,35,35,35	0
4	MG	A	1003	1/1	0.89	0.41	19.65	42,42,42,42	0
4	MG	E	1003	1/1	0.85	0.38	15.13	38,38,38,38	0
2	6PT	G	1001	28/28	0.95	0.20	2.75	27,28,30,30	0
2	6PT	D	1001	28/28	0.95	0.18	2.17	28,29,30,31	0
2	6PT	E	1001	28/28	0.93	0.18	1.94	27,29,30,31	0
2	6PT	B	1001	28/28	0.94	0.18	1.70	28,29,29,29	0
2	6PT	C	1001	28/28	0.93	0.19	1.26	27,29,30,31	0
2	6PT	A	1001	28/28	0.93	0.18	0.50	28,30,31,32	0
2	6PT	F	1001	28/28	0.92	0.17	0.42	29,30,31,32	0
2	6PT	H	1001	28/28	0.95	0.14	-0.10	28,29,30,31	0
3	ZN	C	1002	1/1	0.97	0.12	-0.65	32,32,32,32	0
3	ZN	B	1002	1/1	0.99	0.12	-1.01	29,29,29,29	0
3	ZN	G	1002	1/1	0.98	0.12	-1.30	26,26,26,26	0
3	ZN	D	1002	1/1	0.98	0.10	-1.53	33,33,33,33	0
3	ZN	F	1002	1/1	0.99	0.11	-1.79	37,37,37,37	0
3	ZN	E	1002	1/1	0.99	0.10	-1.83	31,31,31,31	0
3	ZN	H	1002	1/1	0.97	0.08	-1.87	36,36,36,36	0
3	ZN	A	1002	1/1	0.98	0.10	-2.01	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.