Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:21 PM GMT

PDB ID	:	4HYT
Title	:	Na,K-ATPase in the E2P state with bound ouabain and Mg2+ in the cation-binding site
Authors	:	Laursen, M.; Yatime, L.; Nissen, P.; Fedosova, N.U.
Deposited on	:	2012-11-14
Resolution	:	3.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

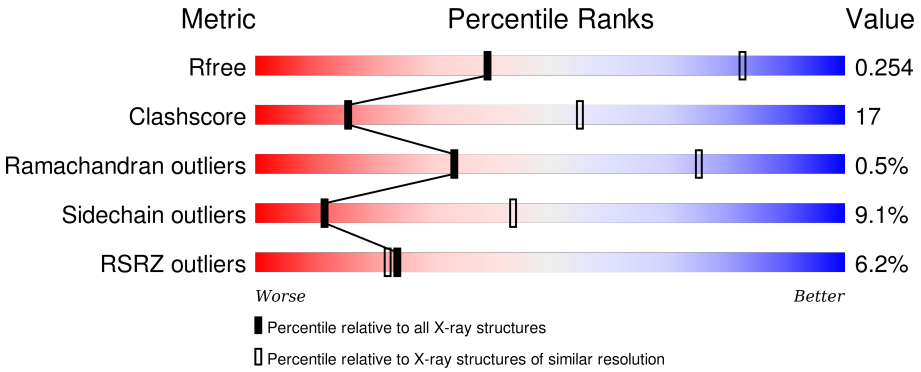
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 >=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 <=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	1021	4% 66% 28%
1	C	1021	8% 67% 27%
2	B	303	5% 51% 37% 7% 5%
2	D	303	7% 50% 38% 6% 5%
3	E	65	32% 15% 51%

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Mol	Chain	Length	Quality of chain
3	G	65	2% 29% 17% 51%

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
10	CE1	A	1110	-	-	-	X
10	CE1	E	2002	-	-	-	X
4	MG	A	1102	-	-	-	X
4	MG	C	2002	-	-	-	X
6	CLR	C	2005	-	-	-	X
9	17F	A	1108	-	-	-	X
9	17F	A	1109	-	-	-	X
9	17F	B	1005	-	-	-	X
9	17F	D	2004	-	-	-	X
9	17F	G	1002	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21220 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			
1	C	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	289	Total	C	N	O	S	0	0	0
			2368	1534	386	435	13			
2	D	287	Total	C	N	O	S	0	0	0
			2349	1519	384	433	13			

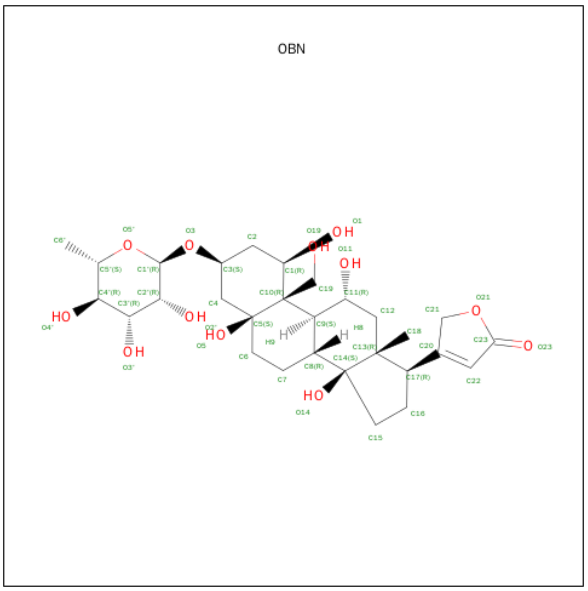
- Molecule 3 is a protein called Na+/K+ ATPase gamma subunit transcript variant a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	32	Total	C	N	O	0	0	0
			255	174	37	44			
3	E	32	Total	C	N	O	0	0	0
			255	174	37	44			

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

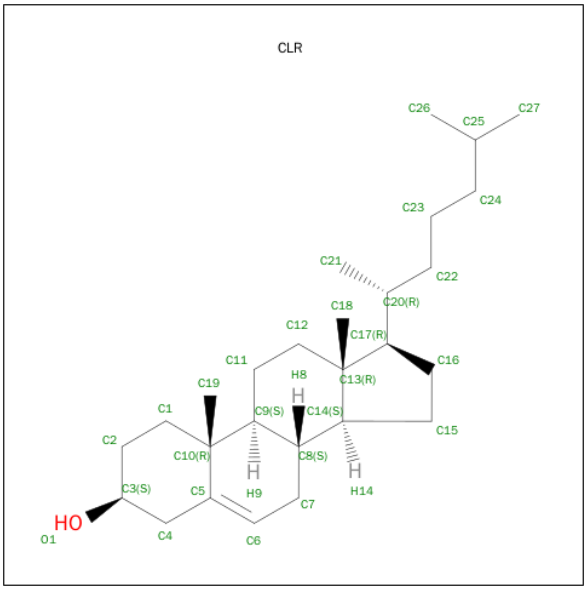
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		
4	C	3	Total	Mg	0	0
			3	3		

- Molecule 5 is OUABAIN (three-letter code: OBN) (formula: $C_{29}H_{44}O_{12}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 41 29 12	0	0
5	C	1	Total C O 41 29 12	0	0

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 28 27 1	0	0
6	G	1	Total C O 28 27 1	0	0

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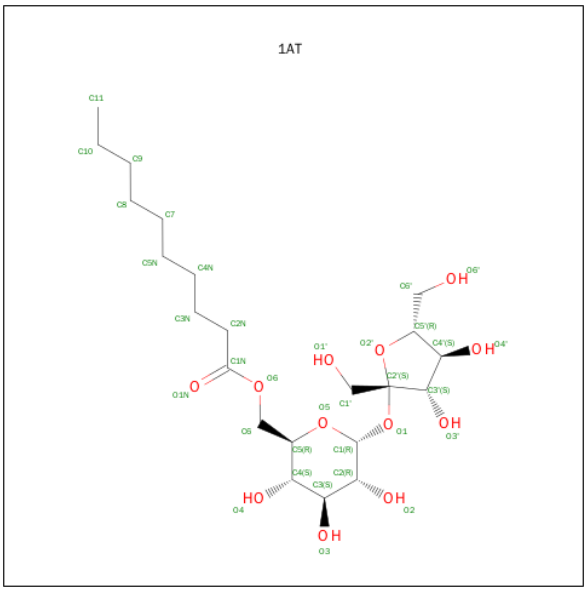
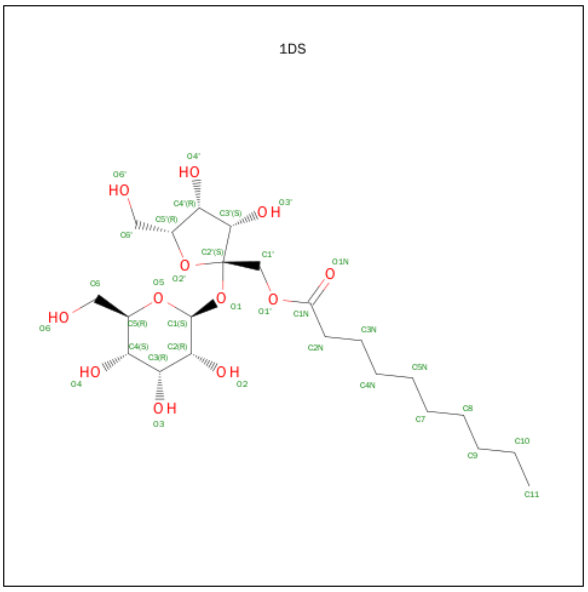
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 28 27 1	0	0
6	E	1	Total C O 28 27 1	0	0

- Molecule 7 is BETA-D-FRUCTOFURANOSYL 6-O-DECANOYL-ALPHA-D-GLUCOPYRANOSIDE (three-letter code: 1AT) (formula: $C_{22}H_{40}O_{12}$).



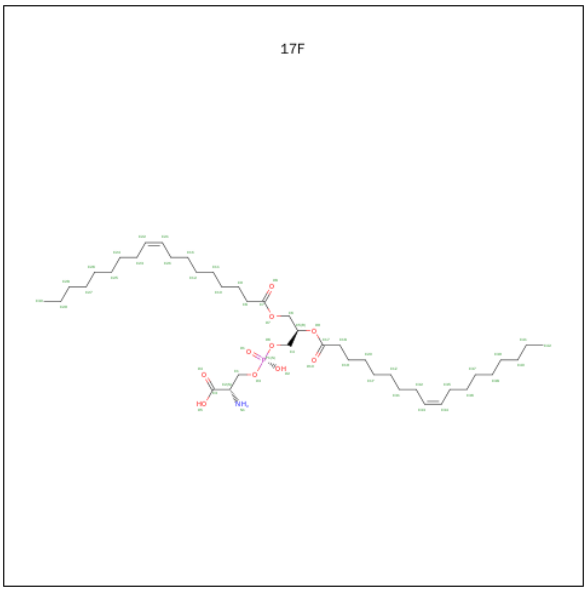
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 29 17 12	0	0

- Molecule 8 is 1-O-DECANOYL-BETA-D-TAGATOFURANOSYL BETA-D-ALLOPYRANOSIDE (three-letter code: 1DS) (formula: $C_{22}H_{40}O_{12}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	29	17	12	0	0

- Molecule 9 is O-[(S)-({(2R)-2,3-BIS[(9Z)-OCTADEC-9-ENOYLOXY]PROPYL}OXY)(HYDROXY)PHOSPHORYL]-L-SERINE (three-letter code: 17F) (formula: $C_{42}H_{78}NO_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	A	1	18	8	1	8	1	0	0
			Total	C	N	O	P		
9	A	1	18	8	1	8	1	0	0

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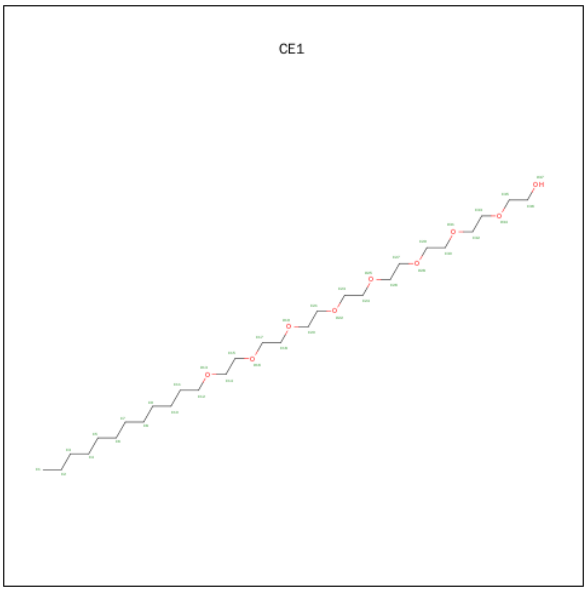
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			24	14	1	8	1		
9	G	1	Total	C	N	O	P	0	0
			27	15	1	10	1		
9	D	1	Total	C	N	O	P	0	0
			28	16	1	10	1		

- Molecule 10 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula: $C_{28}H_{58}O_9$).

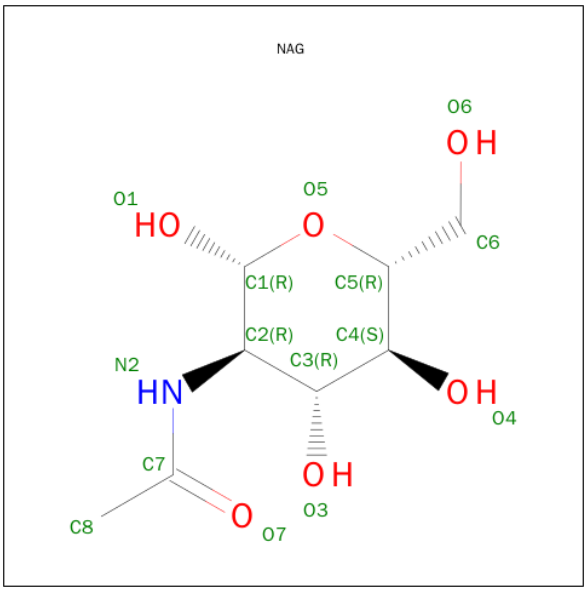


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			34	26	8		
10	E	1	Total	C	O	0	0
			22	18	4		

- Molecule 11 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 12 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C N O 14 8 1 5	0	0
12	B	1	Total C N O 14 8 1 5	0	0
12	D	1	Total C N O 14 8 1 5	0	0
12	D	1	Total C N O 14 8 1 5	0	0
12	D	1	Total C N O 14 8 1 5	0	0

- Molecule 13 is water.

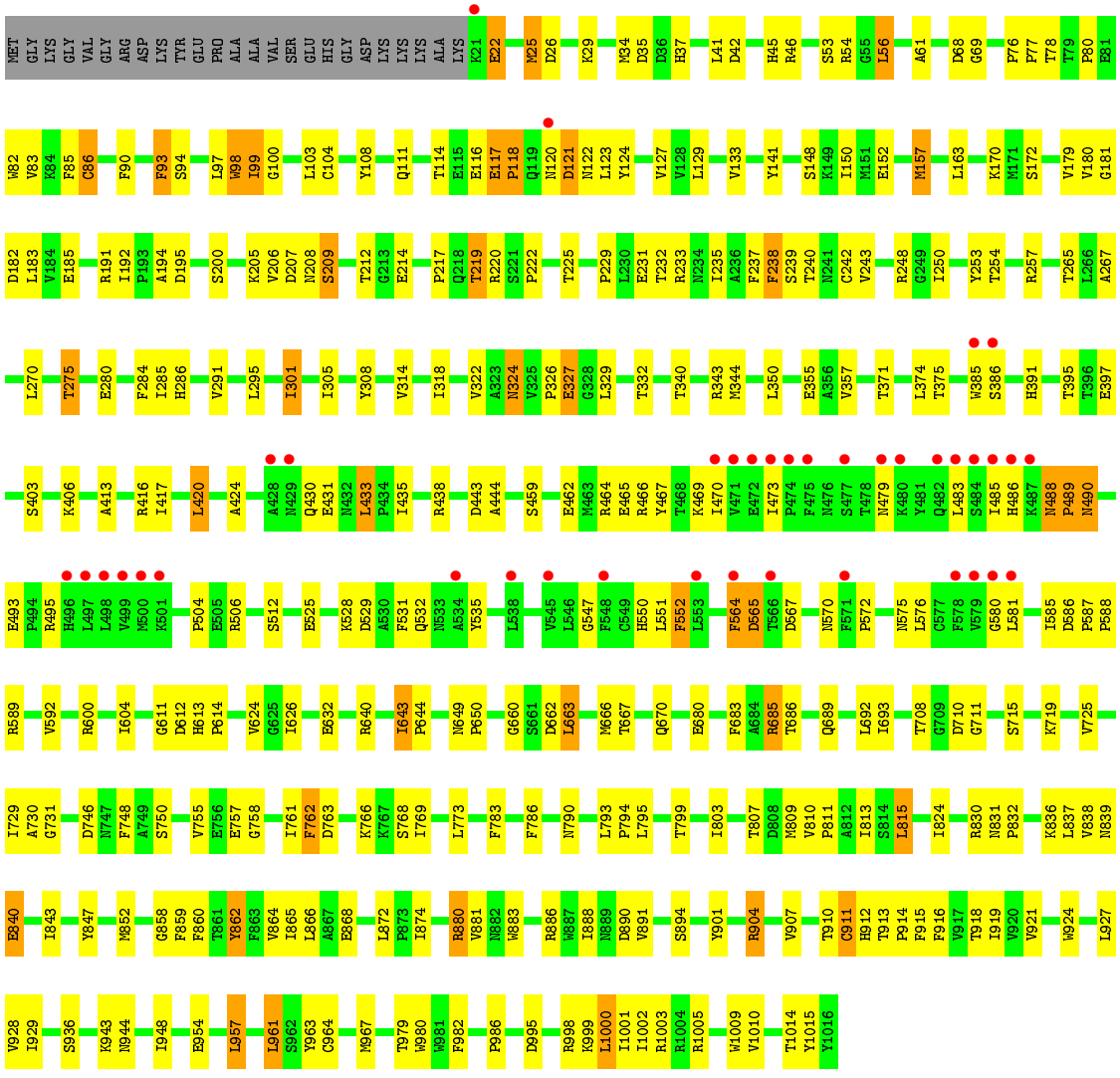
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	3	Total O 3 3	0	0
13	C	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

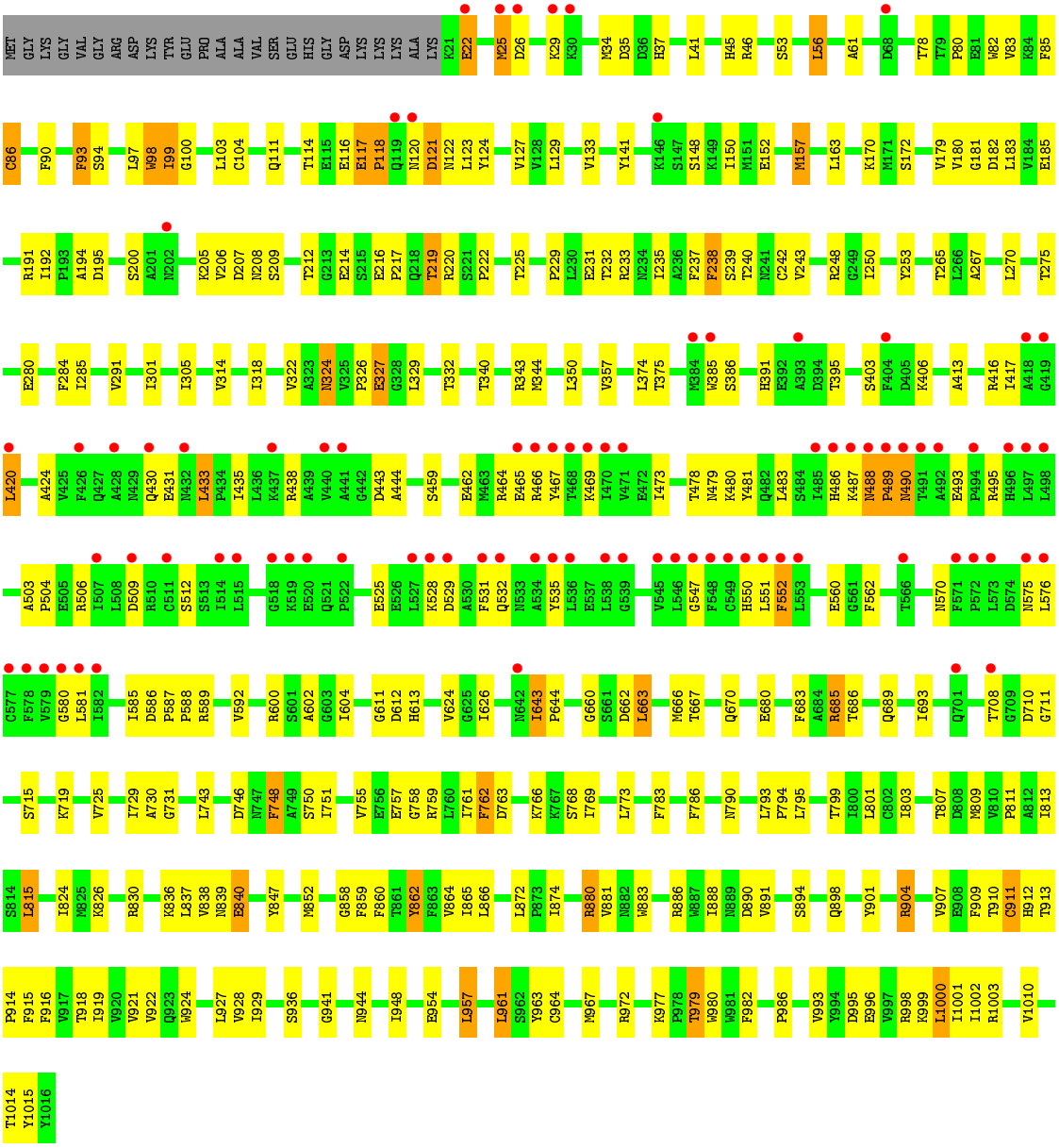
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

Chain A:



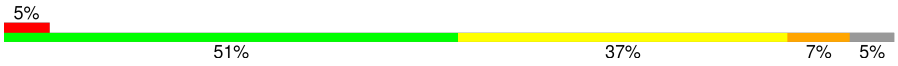
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

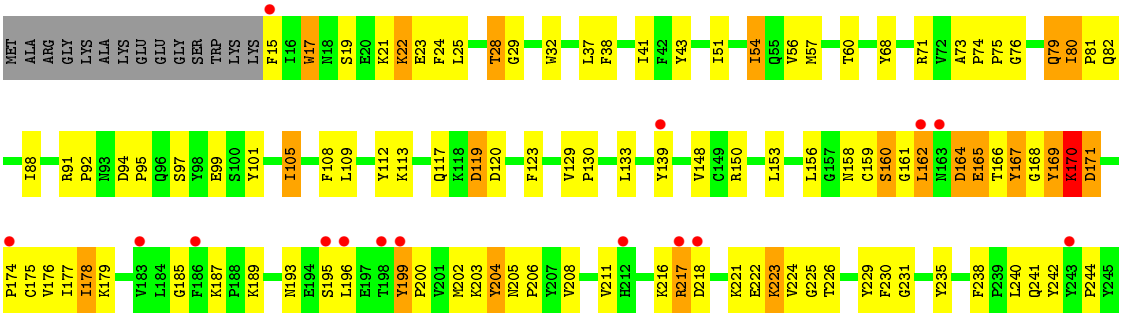
Chain C:

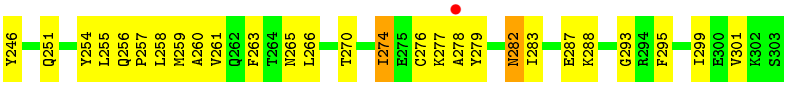


• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain B:

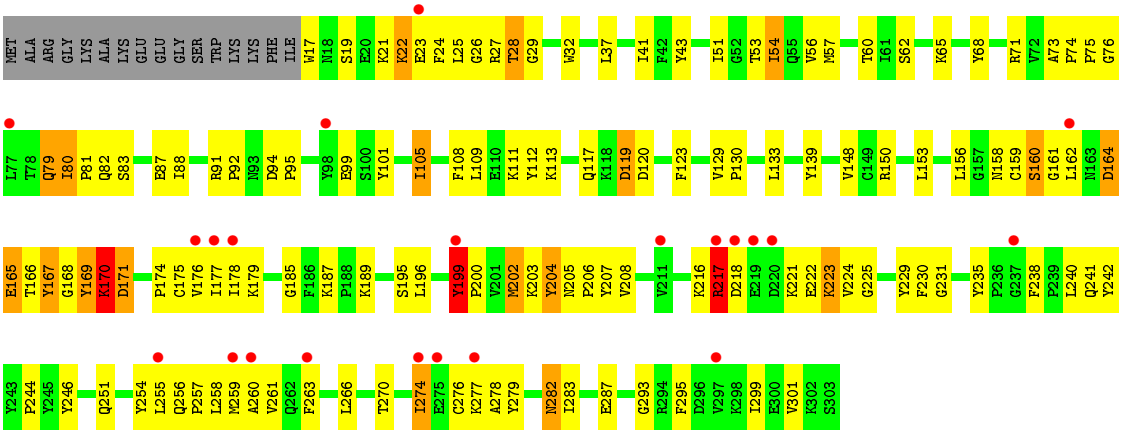






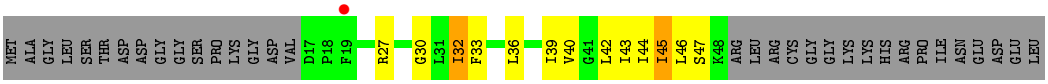
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain D:



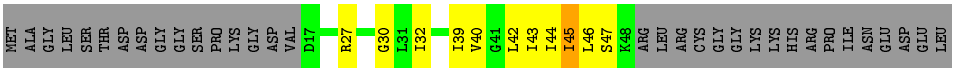
• Molecule 3: Na+/K+ ATPase gamma subunit transcript variant a

Chain G:



• Molecule 3: Na+/K+ ATPase gamma subunit transcript variant a

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.47Å 118.08Å 494.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 3.40 53.88 – 3.40	Depositor EDS
% Data completeness (in resolution range)	75.7 (49.83-3.40) 75.7 (53.88-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.226 , 0.244 0.232 , 0.254	Depositor DCC
R_{free} test set	3603 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	111.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 70.0	EDS
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 72261 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	21220	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: OBN, 1AT, MG, NAG, 17F, PHD, 1DS, CE1, CLR

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	0.31	0/7867	0.53	0/10674
1	C	0.30	0/7867	0.53	0/10674
2	B	0.32	0/2431	0.59	0/3279
2	D	0.34	0/2411	0.59	2/3252 (0.1%)
3	E	0.38	0/261	0.54	0/354
3	G	0.39	0/261	0.55	0/354
All	All	0.31	0/21098	0.54	2/28587 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	D	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	217	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	D	199	TYR	CB-CG-CD2	-5.15	117.91	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	160	SER	Peptide
2	B	165	GLU	Peptide
2	D	160	SER	Peptide
2	D	165	GLU	Peptide

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	7730	0	7777	243	0
1	C	7730	0	7777	226	0
2	B	2368	0	2335	116	0
2	D	2349	0	2315	119	0
3	E	255	0	259	7	0
3	G	255	0	259	9	0
4	A	3	0	0	0	0
4	C	3	0	0	0	0
5	A	41	0	44	10	0
5	C	41	0	44	6	0
6	A	28	0	46	5	0
6	C	28	0	46	2	0
6	E	28	0	46	4	0
6	G	28	0	46	4	0
7	A	29	0	27	6	0
8	A	29	0	27	6	0
9	A	36	0	16	7	0
9	B	24	0	20	2	0
9	D	28	0	22	0	0
9	G	27	0	20	4	0
10	A	34	0	53	18	0
10	E	22	0	37	1	0
11	B	28	0	25	0	0
12	B	28	0	26	0	0
12	D	42	0	39	0	0
13	A	3	0	0	1	0
13	C	3	0	0	0	0
All	All	21220	0	21306	726	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 17.

All (726) 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:A:68:ASP:OD1	1:A:69:GLY:N	1.78	1.15
1:C:794:PRO:HG3	1:C:862:TYR:HE2	1.17	1.07
1:A:794:PRO:HG3	1:A:862:TYR:HE2	1.15	1.07
1:C:794:PRO:HG3	1:C:862:TYR:CE2	1.95	1.00
1:A:794:PRO:HG3	1:A:862:TYR:CE2	1.95	1.00
2:B:199:TYR:HB3	2:B:200:PRO:CD	1.93	0.99
2:D:199:TYR:HB3	2:D:200:PRO:CD	1.95	0.96
1:A:22:GLU:HA	1:A:25:MET:HG3	1.49	0.94
2:D:170:LYS:HB2	2:D:174:PRO:HA	1.51	0.93
2:B:204:TYR:C	2:B:206:PRO:HD2	1.88	0.93
9:B:1005:17F:HN1	9:B:1005:17F:H4A	1.35	0.92
1:C:22:GLU:HA	1:C:25:MET:HG3	1.50	0.92
2:B:170:LYS:HB2	2:B:174:PRO:HA	1.51	0.91
2:D:199:TYR:HB3	2:D:200:PRO:HD2	1.54	0.89
2:B:199:TYR:HB3	2:B:200:PRO:HD2	1.52	0.89
1:A:794:PRO:HB3	1:A:862:TYR:CD2	2.09	0.86
7:A:1106:1AT:H9	1:C:982:PHE:CE2	2.10	0.86
2:B:80:ILE:HG13	2:B:81:PRO:HD3	1.61	0.81
2:D:205:ASN:N	2:D:206:PRO:HD2	1.97	0.80
1:A:1009:TRP:H	10:A:1110:CE1:H271	1.47	0.80
2:D:80:ILE:HG13	2:D:81:PRO:HD3	1.62	0.79
2:D:204:TYR:C	2:D:206:PRO:HD2	2.01	0.79
1:A:111:GLN:HB3	1:A:116:GLU:HG2	1.65	0.79
2:D:204:TYR:O	2:D:208:VAL:HG12	1.83	0.78
1:C:864:VAL:HG22	2:D:57:MET:HG3	1.64	0.78
1:C:111:GLN:HB3	1:C:116:GLU:HG2	1.65	0.78
2:B:204:TYR:O	2:B:208:VAL:HG12	1.84	0.77
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.65	0.77
2:B:217:ARG:HH11	2:B:217:ARG:HG2	1.50	0.76
2:B:216:LYS:HB2	2:B:221:LYS:HG2	1.67	0.76
2:D:148:VAL:HG11	2:D:254:TYR:HA	1.67	0.76
2:D:216:LYS:HB2	2:D:221:LYS:HG2	1.66	0.76
1:A:116:GLU:HG3	1:A:118:PRO:HD2	1.66	0.75
2:D:217:ARG:HH11	2:D:217:ARG:HG2	1.51	0.75
2:D:129:VAL:HG22	2:D:204:TYR:OH	1.87	0.75
2:B:148:VAL:HG11	2:B:254:TYR:HA	1.67	0.75
10:A:1110:CE1:H272	10:A:1110:CE1:H212	1.68	0.75
2:B:205:ASN:N	2:B:206:PRO:HD2	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1110:CE1:H211	10:A:1110:CE1:H152	1.67	0.75
1:C:116:GLU:HG3	1:C:118:PRO:HD2	1.66	0.75
1:C:862:TYR:HE1	1:C:866:LEU:HD12	1.52	0.74
9:A:1108:17F:O1	9:A:1109:17F:H4	1.88	0.74
1:A:1009:TRP:HB3	10:A:1110:CE1:H242	1.69	0.74
2:D:88:ILE:HB	2:D:299:ILE:HG22	1.70	0.74
8:A:1107:1DS:H18	1:C:941:GLY:HA3	1.70	0.73
1:C:794:PRO:HB3	1:C:862:TYR:CD2	2.24	0.73
2:B:88:ILE:HB	2:B:299:ILE:HG22	1.69	0.72
7:A:1106:1AT:H9	1:C:982:PHE:HE2	1.53	0.72
1:A:840:GLU:HA	9:A:1108:17F:H4A	1.70	0.72
2:B:168:GLY:HA3	2:B:171:ASP:HB3	1.72	0.72
1:A:862:TYR:HE1	1:A:866:LEU:HD12	1.54	0.72
2:B:130:PRO:HB2	2:B:204:TYR:CE1	2.26	0.71
2:D:204:TYR:HD2	2:D:235:TYR:CZ	2.08	0.71
1:C:865:ILE:HD12	1:C:914:PRO:HG3	1.73	0.71
1:A:865:ILE:HD12	1:A:914:PRO:HG3	1.73	0.70
1:C:195:ASP:HB2	1:C:253:TYR:HB2	1.73	0.70
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.73	0.70
3:E:45:ILE:HD12	3:E:46:LEU:HG	1.73	0.70
2:D:204:TYR:CD2	2:D:235:TYR:CZ	2.79	0.70
2:D:168:GLY:HA3	2:D:171:ASP:HB3	1.72	0.69
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.75	0.69
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.73	0.69
1:C:385:TRP:HB3	1:C:581:LEU:H	1.58	0.69
1:A:385:TRP:HB3	1:A:581:LEU:H	1.58	0.68
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.76	0.68
1:C:786:PHE:CZ	5:C:2004:OBN:H6'1	2.29	0.68
1:C:890:ASP:OD1	2:D:82:GLN:NE2	2.26	0.68
2:D:113:LYS:HA	2:D:153:LEU:HD11	1.75	0.67
1:A:907:VAL:HA	1:A:910:THR:HG22	1.77	0.67
2:B:165:GLU:HB3	2:B:166:THR:HA	1.76	0.67
10:A:1110:CE1:H92	2:B:38:PHE:HD1	1.59	0.67
2:D:80:ILE:HD11	2:D:176:VAL:HA	1.77	0.67
2:D:216:LYS:H	2:D:221:LYS:HD2	1.60	0.67
1:A:565:ASP:O	1:A:570:ASN:ND2	2.26	0.67
2:D:165:GLU:HB3	2:D:166:THR:HA	1.76	0.67
1:C:907:VAL:HA	1:C:910:THR:HG22	1.77	0.67
2:B:205:ASN:N	2:B:206:PRO:CD	2.59	0.66
3:G:45:ILE:HD12	3:G:46:LEU:HG	1.75	0.66
2:B:216:LYS:H	2:B:221:LYS:HD2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:GLU:OE2	9:A:1108:17F:N1	2.28	0.66
1:A:794:PRO:HB3	1:A:862:TYR:HD2	1.59	0.65
2:B:80:ILE:HD11	2:B:176:VAL:HA	1.77	0.65
1:A:375:THR:HA	1:A:588:PRO:HA	1.79	0.65
2:B:29:GLY:HA2	2:B:32:TRP:CD1	2.31	0.65
1:C:550:HIS:HE2	1:C:552:PHE:HE1	1.44	0.65
1:A:212:THR:HG23	1:A:214:GLU:H	1.62	0.65
2:D:130:PRO:HB2	2:D:204:TYR:CE1	2.32	0.65
2:D:29:GLY:HA2	2:D:32:TRP:CD1	2.31	0.65
2:D:205:ASN:N	2:D:206:PRO:CD	2.61	0.64
1:C:592:VAL:HG22	1:C:748:PHE:HD2	1.62	0.64
2:D:24:PHE:HB3	2:D:28:THR:HA	1.80	0.64
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.62	0.64
2:D:189:LYS:H	2:D:282:ASN:HB2	1.63	0.64
1:A:275:THR:OG1	1:A:355:GLU:OE2	2.16	0.64
1:A:430:GLN:HG3	1:A:433:LEU:HD13	1.79	0.64
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.63	0.64
1:C:604:ILE:HD11	1:C:755:VAL:HG21	1.80	0.64
1:A:550:HIS:HE2	1:A:552:PHE:HE1	1.45	0.63
1:C:430:GLN:HG3	1:C:433:LEU:HD13	1.80	0.63
2:B:189:LYS:H	2:B:282:ASN:HB2	1.63	0.63
1:A:1001:ILE:HG22	1:A:1010:VAL:HG21	1.81	0.63
1:A:1009:TRP:H	10:A:1110:CE1:C27	2.11	0.63
1:C:624:VAL:HG23	1:C:626:ILE:HG13	1.81	0.63
2:B:24:PHE:HB3	2:B:28:THR:HA	1.79	0.62
1:C:208:ASN:HB3	1:C:212:THR:HG22	1.82	0.62
8:A:1107:1DS:H14	8:A:1107:1DS:H16	1.48	0.62
1:C:212:THR:HG23	1:C:214:GLU:H	1.64	0.62
1:A:632:GLU:OE1	1:A:640:ARG:NH1	2.33	0.61
1:A:270:LEU:HB2	1:A:719:LYS:HG2	1.82	0.61
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.35	0.61
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.35	0.61
1:A:790:ASN:OD1	1:A:880:ARG:NH1	2.31	0.61
1:C:790:ASN:OD1	1:C:880:ARG:NH1	2.31	0.60
1:A:208:ASN:HB3	1:A:212:THR:HG22	1.82	0.60
2:D:158:ASN:O	2:D:166:THR:OG1	2.19	0.60
1:C:589:ARG:HB2	1:C:592:VAL:HG23	1.82	0.60
1:C:375:THR:HA	1:C:588:PRO:HA	1.83	0.60
2:D:76:GLY:HA2	2:D:293:GLY:H	1.67	0.60
1:A:624:VAL:HG23	1:A:626:ILE:HG13	1.82	0.60
2:D:80:ILE:HD12	2:D:105:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:LYS:O	2:D:23:GLU:HA	2.02	0.60
1:C:117:GLU:HG3	1:C:118:PRO:HD3	1.83	0.60
1:C:1001:ILE:HG22	1:C:1010:VAL:HG21	1.83	0.60
2:B:21:LYS:O	2:B:23:GLU:HA	2.02	0.60
1:A:604:ILE:HD11	1:A:755:VAL:HG21	1.83	0.60
3:G:36:LEU:HD12	9:G:1002:17F:C18	2.32	0.60
2:B:80:ILE:HD12	2:B:105:ILE:HD12	1.83	0.60
1:A:371:THR:O	1:A:710:ASP:OD2	2.20	0.60
2:D:179:LYS:HD2	2:D:256:GLN:HE21	1.66	0.60
1:A:529:ASP:HA	1:A:532:GLN:HB2	1.84	0.60
2:B:166:THR:HB	2:B:169:TYR:H	1.68	0.59
1:C:786:PHE:HZ	5:C:2004:OBN:H6'1	1.67	0.59
2:B:130:PRO:HA	2:B:241:GLN:NE2	2.17	0.59
2:D:166:THR:HB	2:D:169:TYR:H	1.68	0.59
2:D:130:PRO:HA	2:D:241:GLN:NE2	2.17	0.59
2:B:25:LEU:H	2:B:29:GLY:HA3	1.67	0.59
2:D:25:LEU:H	2:D:29:GLY:HA3	1.67	0.59
1:C:163:LEU:HD23	1:C:185:GLU:HB3	1.84	0.59
1:C:529:ASP:HA	1:C:532:GLN:HB2	1.84	0.59
1:A:589:ARG:HB2	1:A:592:VAL:HG23	1.85	0.59
1:A:117:GLU:HG3	1:A:118:PRO:HD3	1.83	0.59
1:C:430:GLN:HB3	1:C:438:ARG:HD3	1.85	0.59
3:G:40:VAL:O	3:G:44:ILE:HG12	2.03	0.59
2:B:79:GLN:HB3	2:B:295:PHE:CE1	2.38	0.59
2:B:179:LYS:HD2	2:B:256:GLN:HE21	1.67	0.59
2:D:217:ARG:NH1	2:D:218:ASP:OD2	2.36	0.58
2:B:199:TYR:CB	2:B:200:PRO:CD	2.71	0.58
2:B:217:ARG:NH1	2:B:218:ASP:OD2	2.36	0.58
2:D:222:GLU:OE1	2:D:222:GLU:N	2.26	0.58
1:C:794:PRO:CG	1:C:862:TYR:CE2	2.81	0.58
2:B:204:TYR:HD2	2:B:235:TYR:CZ	2.21	0.58
1:A:840:GLU:HG3	9:A:1108:17F:P1	2.43	0.58
1:A:551:LEU:HD22	1:A:576:LEU:HD23	1.86	0.58
2:B:119:ASP:O	2:B:123:PHE:HB2	2.03	0.58
2:D:22:LYS:HG2	2:D:23:GLU:HG3	1.85	0.58
1:A:163:LEU:HD23	1:A:185:GLU:HB3	1.84	0.58
1:A:794:PRO:CG	1:A:862:TYR:CE2	2.78	0.58
2:D:160:SER:O	2:D:162:LEU:N	2.37	0.58
1:A:512:SER:HB3	1:A:575:ASN:HA	1.86	0.58
2:B:158:ASN:O	2:B:166:THR:OG1	2.21	0.57
1:A:880:ARG:HA	1:A:883:TRP:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:LEU:HD21	1:C:327:GLU:HG2	1.86	0.57
2:B:225:GLY:HA2	2:B:266:LEU:HD23	1.85	0.57
1:C:512:SER:HB3	1:C:575:ASN:HA	1.86	0.57
1:C:880:ARG:HA	1:C:883:TRP:HB3	1.85	0.57
1:C:551:LEU:HD22	1:C:576:LEU:HD23	1.86	0.57
1:A:807:THR:HB	1:A:954:GLU:HG3	1.86	0.57
1:A:238:PHE:HD1	1:A:239:SER:N	2.03	0.57
1:C:343:ARG:NH2	1:C:757:GLU:OE1	2.38	0.57
1:A:943:LYS:HE3	7:A:1106:1AT:H25	1.87	0.57
2:B:76:GLY:HA2	2:B:293:GLY:H	1.68	0.57
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.86	0.57
2:D:225:GLY:HA2	2:D:266:LEU:HD23	1.86	0.57
1:C:807:THR:HB	1:C:954:GLU:HG3	1.86	0.57
1:A:200:SER:HA	1:A:222:PRO:HG3	1.87	0.57
2:D:79:GLN:HB3	2:D:295:PHE:CE1	2.39	0.57
1:C:794:PRO:HB3	1:C:862:TYR:HD2	1.69	0.57
5:A:1104:OBN:H3	5:A:1104:OBN:H5'	1.87	0.57
1:A:430:GLN:HB3	1:A:438:ARG:HD3	1.85	0.56
3:E:40:VAL:O	3:E:44:ILE:HG12	2.06	0.56
1:C:478:THR:O	1:C:506:ARG:NH1	2.39	0.56
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.87	0.56
1:C:443:ASP:OD1	1:C:444:ALA:N	2.35	0.56
1:A:94:SER:HB3	1:A:133:VAL:HG13	1.88	0.56
2:B:22:LYS:HG2	2:B:23:GLU:HG3	1.86	0.56
1:C:329:LEU:HD11	1:C:769:ILE:HA	1.88	0.56
1:C:238:PHE:HD1	1:C:239:SER:N	2.03	0.56
2:B:204:TYR:CD2	2:B:235:TYR:CZ	2.93	0.56
2:D:119:ASP:O	2:D:123:PHE:HB2	2.05	0.56
1:A:329:LEU:HD11	1:A:769:ILE:HA	1.87	0.56
1:A:118:PRO:HB3	1:A:122:ASN:H	1.71	0.55
1:A:860:PHE:HZ	6:A:1105:CLR:H191	1.70	0.55
10:A:1110:CE1:H92	2:B:38:PHE:CD1	2.41	0.55
2:B:80:ILE:CG1	2:B:81:PRO:HD3	2.36	0.55
1:A:443:ASP:OD1	1:A:444:ALA:N	2.37	0.55
1:A:585:ILE:HG13	1:A:586:ASP:N	2.21	0.55
2:B:160:SER:O	2:B:162:LEU:N	2.39	0.55
1:A:888:ILE:O	1:A:904:ARG:NH2	2.40	0.55
1:A:683:PHE:HB3	1:A:686:THR:HG21	1.89	0.55
1:C:94:SER:HB3	1:C:133:VAL:HG13	1.88	0.55
1:A:685:ARG:NH1	1:A:685:ARG:HB3	2.22	0.54
1:C:469:LYS:HA	1:C:486:HIS:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ASN:ND2	1:A:493:GLU:O	2.40	0.54
1:C:118:PRO:HB3	1:C:122:ASN:H	1.72	0.54
2:B:278:ALA:O	2:B:283:ILE:HG21	2.08	0.54
1:A:291:VAL:HG21	1:A:847:TYR:HE2	1.73	0.54
1:C:488:ASN:ND2	1:C:493:GLU:O	2.41	0.54
1:C:683:PHE:HB3	1:C:686:THR:HG21	1.89	0.54
3:G:39:ILE:O	3:G:43:ILE:HG12	2.08	0.54
1:C:999:LYS:O	1:C:1003:ARG:HG3	2.08	0.54
2:D:278:ALA:O	2:D:283:ILE:HG21	2.07	0.54
1:C:890:ASP:OD1	1:C:890:ASP:N	2.41	0.54
1:C:909:PHE:HE2	1:C:972:ARG:CZ	2.21	0.54
1:C:710:ASP:OD1	1:C:711:GLY:N	2.40	0.54
1:C:200:SER:HA	1:C:222:PRO:HG3	1.89	0.54
1:C:888:ILE:O	1:C:904:ARG:NH2	2.40	0.54
1:A:329:LEU:HA	1:A:332:THR:OG1	2.06	0.54
1:A:343:ARG:NH2	1:A:757:GLU:OE1	2.41	0.54
1:C:585:ILE:HG13	1:C:586:ASP:N	2.22	0.54
1:C:961:LEU:HD23	1:C:967:MET:HE1	1.90	0.54
1:A:890:ASP:N	1:A:890:ASP:OD1	2.41	0.54
2:D:170:LYS:HB2	2:D:174:PRO:CA	2.34	0.54
10:A:1110:CE1:H321	10:A:1110:CE1:H182	1.90	0.54
6:C:2005:CLR:H212	2:D:53:THR:HA	1.90	0.54
1:A:710:ASP:OD1	1:A:711:GLY:N	2.41	0.53
1:C:1000:LEU:HD23	1:C:1003:ARG:NH2	2.22	0.53
1:C:37:HIS:HB3	1:C:235:ILE:HD11	1.90	0.53
1:A:267:ALA:HB2	1:A:715:SER:HB3	1.91	0.53
1:A:469:LYS:HA	1:A:486:HIS:CD2	2.43	0.53
1:A:963:TYR:O	3:G:27:ARG:HG3	2.09	0.53
1:A:42:ASP:OD1	1:A:46:ARG:NH1	2.41	0.53
2:D:101:TYR:O	2:D:105:ILE:HG12	2.09	0.53
1:C:469:LYS:HA	1:C:486:HIS:HD2	1.73	0.53
1:A:662:ASP:O	1:A:666:MET:HG3	2.09	0.53
3:E:39:ILE:O	3:E:43:ILE:HG12	2.08	0.53
7:A:1106:1AT:H20	1:C:979:THR:H	1.74	0.53
1:C:662:ASP:O	1:C:666:MET:HG3	2.09	0.53
1:C:685:ARG:NH1	1:C:685:ARG:HB3	2.24	0.52
10:A:1110:CE1:H81	2:B:41:ILE:HG21	1.90	0.52
1:A:982:PHE:CE2	8:A:1107:1DS:H24	2.44	0.52
2:B:179:LYS:HD2	2:B:256:GLN:NE2	2.25	0.52
1:C:395:THR:HB	1:C:587:PRO:HB3	1.92	0.52
2:B:101:TYR:O	2:B:105:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:LEU:HD23	1:A:1003:ARG:NH2	2.24	0.52
1:C:963:TYR:O	3:E:27:ARG:HG3	2.10	0.52
1:C:550:HIS:NE2	1:C:552:PHE:HE1	2.08	0.52
2:D:179:LYS:HD2	2:D:256:GLN:NE2	2.24	0.52
1:C:329:LEU:HA	1:C:332:THR:OG1	2.10	0.52
1:C:995:ASP:OD1	1:C:998:ARG:NH1	2.42	0.52
1:A:395:THR:HB	1:A:587:PRO:HB3	1.92	0.52
1:A:551:LEU:HG	1:A:552:PHE:O	2.10	0.51
1:A:999:LYS:O	1:A:1003:ARG:HG3	2.10	0.51
2:D:120:ASP:OD1	2:D:150:ARG:NH2	2.43	0.51
1:A:25:MET:O	1:A:29:LYS:HG3	2.11	0.51
1:C:977:LYS:HD3	2:D:68:TYR:CZ	2.45	0.51
2:B:242:TYR:CD2	2:B:257:PRO:HG3	2.45	0.51
2:B:120:ASP:OD1	2:B:150:ARG:NH2	2.44	0.51
2:B:166:THR:N	2:B:167:TYR:HA	2.25	0.51
2:D:153:LEU:H	2:D:153:LEU:HD12	1.76	0.51
9:G:1002:17F:H5	3:E:44:ILE:HD12	1.91	0.51
2:D:205:ASN:OD1	2:D:206:PRO:HD3	2.10	0.51
1:C:104:CYS:SG	1:C:322:VAL:HG11	2.51	0.51
2:D:166:THR:N	2:D:167:TYR:HA	2.25	0.51
1:A:643:ILE:HG22	1:A:644:PRO:HD2	1.93	0.51
1:C:206:VAL:HA	1:C:242:CYS:HA	1.93	0.51
1:A:117:GLU:OE2	5:A:1104:OBN:O5	2.28	0.51
1:A:995:ASP:OD1	1:A:998:ARG:NH1	2.43	0.51
1:A:469:LYS:HA	1:A:486:HIS:HD2	1.75	0.51
1:A:467:TYR:CZ	1:A:489:PRO:HG3	2.46	0.51
2:D:242:TYR:CD2	2:D:257:PRO:HG3	2.45	0.51
1:C:467:TYR:CZ	1:C:489:PRO:HG3	2.46	0.50
1:A:206:VAL:HA	1:A:242:CYS:HA	1.93	0.50
2:B:216:LYS:HG3	2:B:221:LYS:HA	1.93	0.50
1:C:551:LEU:HG	1:C:552:PHE:O	2.10	0.50
1:C:103:LEU:HB3	1:C:318:ILE:HG23	1.93	0.50
1:A:852:MET:HG2	2:B:43:TYR:CE2	2.45	0.50
1:A:284:PHE:HE1	1:A:773:LEU:HD11	1.76	0.50
1:C:852:MET:HG2	2:D:43:TYR:CE2	2.46	0.50
1:A:547:GLY:HA2	1:A:581:LEU:HD23	1.93	0.50
2:B:153:LEU:H	2:B:153:LEU:HD12	1.75	0.50
2:B:204:TYR:HB2	2:B:235:TYR:CE1	2.47	0.50
1:A:963:TYR:CE2	6:G:1001:CLR:H6	2.46	0.50
1:A:485:ILE:HD13	1:A:564:PHE:CZ	2.46	0.50
1:C:862:TYR:CE1	1:C:866:LEU:HD12	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1010:VAL:HG13	10:A:1110:CE1:H241	1.92	0.50
1:C:181:GLY:HA2	1:C:250:ILE:HG23	1.93	0.50
1:A:550:HIS:NE2	1:A:552:PHE:HE1	2.09	0.50
1:C:667:THR:N	1:C:670:GLN:OE1	2.43	0.50
2:B:92:PRO:HG3	2:B:301:VAL:HG12	1.93	0.50
1:A:192:ILE:HG12	1:A:240:THR:O	2.12	0.50
1:A:551:LEU:HD13	1:A:576:LEU:HA	1.94	0.50
2:D:133:LEU:HG	2:D:240:LEU:HB3	1.94	0.50
1:C:267:ALA:HB2	1:C:715:SER:HB3	1.93	0.50
2:B:222:GLU:N	2:B:222:GLU:OE1	2.27	0.50
1:C:551:LEU:HD13	1:C:576:LEU:HA	1.94	0.50
1:C:270:LEU:HB2	1:C:719:LYS:HG2	1.93	0.50
1:A:858:GLY:HA2	1:A:918:THR:HG21	1.94	0.50
1:C:725:VAL:HG11	1:C:751:ILE:HD11	1.93	0.50
2:D:80:ILE:CG1	2:D:81:PRO:HD3	2.37	0.50
1:A:880:ARG:NH2	5:A:1104:OBN:C6'	2.75	0.50
1:A:525:GLU:HA	1:A:528:LYS:HB3	1.94	0.50
1:C:291:VAL:HG21	1:C:847:TYR:HE2	1.77	0.50
1:C:963:TYR:CE2	6:E:2001:CLR:H6	2.47	0.49
1:C:547:GLY:HA2	1:C:581:LEU:HD23	1.94	0.49
1:C:592:VAL:HG22	1:C:748:PHE:CD2	2.46	0.49
1:C:301:ILE:O	1:C:305:ILE:HG12	2.12	0.49
1:C:192:ILE:HG12	1:C:240:THR:O	2.12	0.49
1:A:799:THR:HG21	1:A:912:HIS:HB3	1.93	0.49
5:A:1104:OBN:O1	5:A:1104:OBN:O3	2.25	0.49
1:A:862:TYR:CE1	1:A:866:LEU:HD12	2.42	0.49
2:D:276:CYS:HB2	2:D:295:PHE:HD2	1.76	0.49
1:C:795:LEU:HD13	1:C:915:PHE:HB3	1.94	0.49
1:A:181:GLY:HA2	1:A:250:ILE:HG23	1.93	0.49
1:C:858:GLY:HA2	1:C:918:THR:HG21	1.93	0.49
1:C:552:PHE:CD1	1:C:552:PHE:N	2.80	0.49
2:B:276:CYS:HB2	2:B:295:PHE:HD2	1.77	0.49
1:C:284:PHE:CD1	1:C:838:VAL:HG21	2.47	0.49
1:C:479:ASN:HB3	1:C:481:TYR:CE2	2.48	0.49
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.93	0.49
1:A:118:PRO:C	1:A:121:ASP:H	2.15	0.49
1:A:552:PHE:CD1	1:A:552:PHE:N	2.81	0.49
2:B:51:ILE:O	2:B:54:ILE:HG22	2.12	0.49
1:A:874:ILE:H	1:A:874:ILE:HD12	1.77	0.49
1:C:643:ILE:HG22	1:C:644:PRO:HD2	1.93	0.49
1:C:98:TRP:CE2	1:C:133:VAL:HG11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:PHE:O	1:C:240:THR:OG1	2.26	0.49
5:C:2004:OBN:H5'	5:C:2004:OBN:H3	1.93	0.49
2:D:153:LEU:HB2	2:D:162:LEU:HD23	1.94	0.49
2:D:92:PRO:HG3	2:D:301:VAL:HG12	1.93	0.49
1:A:83:VAL:O	1:A:86:CYS:HB2	2.13	0.49
2:B:133:LEU:HG	2:B:240:LEU:HB3	1.95	0.49
2:D:199:TYR:CB	2:D:200:PRO:CD	2.70	0.49
2:B:80:ILE:HG12	2:B:177:ILE:H	1.78	0.49
1:C:763:ASP:O	1:C:766:LYS:HB2	2.13	0.49
1:A:880:ARG:HH21	5:A:1104:OBN:H6'3	1.78	0.49
1:A:795:LEU:HD13	1:A:915:PHE:HB3	1.95	0.49
2:D:204:TYR:CD2	2:D:235:TYR:CE2	3.01	0.48
1:A:872:LEU:HD23	1:A:894:SER:HB2	1.94	0.48
1:A:301:ILE:O	1:A:305:ILE:HG12	2.13	0.48
2:D:204:TYR:HB2	2:D:235:TYR:CE1	2.47	0.48
1:C:799:THR:HG21	1:C:912:HIS:HB3	1.94	0.48
1:A:794:PRO:CB	1:A:862:TYR:CD2	2.89	0.48
2:D:216:LYS:HG3	2:D:221:LYS:HA	1.95	0.48
1:A:284:PHE:CD1	1:A:838:VAL:HG21	2.48	0.48
1:C:217:PRO:HB3	1:C:243:VAL:HG21	1.95	0.48
1:A:809:MET:O	1:A:813:ILE:HG12	2.13	0.48
1:A:98:TRP:CE2	1:A:133:VAL:HG11	2.48	0.48
1:A:891:VAL:HG21	1:A:904:ARG:NH1	2.29	0.48
1:C:872:LEU:HD23	1:C:894:SER:HB2	1.94	0.48
2:B:170:LYS:HB2	2:B:174:PRO:CA	2.33	0.48
1:C:891:VAL:HG21	1:C:904:ARG:NH1	2.29	0.48
1:A:880:ARG:NH2	5:A:1104:OBN:H6'2	2.29	0.48
1:A:99:ILE:HG13	1:A:100:GLY:N	2.28	0.48
1:A:961:LEU:HD23	1:A:967:MET:HE1	1.95	0.48
1:C:29:LYS:HE2	1:C:265:THR:HB	1.96	0.48
1:C:403:SER:OG	1:C:406:LYS:NZ	2.47	0.48
1:A:217:PRO:HB3	1:A:243:VAL:HG21	1.96	0.48
1:A:794:PRO:HG2	1:A:859:PHE:HE1	1.78	0.48
1:A:291:VAL:HG21	1:A:847:TYR:CE2	2.48	0.48
1:A:915:PHE:O	1:A:919:ILE:HG12	2.14	0.48
2:B:95:PRO:O	2:B:99:GLU:HG2	2.14	0.48
1:A:1009:TRP:H	10:A:1110:CE1:H262	1.78	0.48
1:A:116:GLU:HG3	1:A:118:PRO:CD	2.40	0.48
1:C:525:GLU:HA	1:C:528:LYS:HB3	1.95	0.48
1:C:118:PRO:C	1:C:121:ASP:H	2.16	0.47
1:C:284:PHE:HE1	1:C:773:LEU:HD11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:SER:OG	1:A:406:LYS:NZ	2.47	0.47
1:A:237:PHE:O	1:A:240:THR:OG1	2.24	0.47
1:A:41:LEU:H	1:A:41:LEU:HD12	1.79	0.47
7:A:1106:1AT:O1N	7:A:1106:1AT:O4	2.32	0.47
2:D:80:ILE:HG12	2:D:177:ILE:H	1.79	0.47
2:B:73:ALA:O	2:B:75:PRO:HD3	2.15	0.47
1:A:929:ILE:HB	1:A:995:ASP:OD2	2.14	0.47
1:C:874:ILE:H	1:C:874:ILE:HD12	1.78	0.47
1:C:836:LYS:HB2	1:C:839:ASN:HB3	1.96	0.47
2:D:263:PHE:CE1	2:D:274:ILE:HG13	2.49	0.47
1:A:667:THR:N	1:A:670:GLN:OE1	2.42	0.47
1:C:479:ASN:HB3	1:C:481:TYR:CD2	2.49	0.47
1:C:689:GLN:O	1:C:693:ILE:HG12	2.14	0.47
1:A:708:THR:HG22	1:A:725:VAL:HB	1.96	0.47
1:C:612:ASP:OD1	1:C:613:HIS:N	2.40	0.47
1:C:99:ILE:HG13	1:C:100:GLY:N	2.29	0.47
1:A:1009:TRP:N	10:A:1110:CE1:H262	2.29	0.47
2:D:73:ALA:O	2:D:75:PRO:HD3	2.15	0.47
1:C:83:VAL:O	1:C:86:CYS:HB2	2.13	0.47
1:C:809:MET:O	1:C:813:ILE:HG12	2.14	0.47
2:D:244:PRO:HG2	2:D:246:TYR:CE1	2.50	0.47
1:A:944:ASN:O	1:A:948:ILE:HG12	2.14	0.47
1:C:386:SER:HB2	1:C:391:HIS:NE2	2.29	0.47
2:B:129:VAL:HG22	2:B:204:TYR:OH	2.15	0.47
2:D:230:PHE:HD2	2:D:260:ALA:HB3	1.80	0.47
3:G:32:ILE:HG22	9:G:1002:17F:O10	2.15	0.47
1:A:416:ARG:NH1	1:A:467:TYR:OH	2.37	0.47
1:A:666:MET:HE3	1:A:670:GLN:HB3	1.96	0.47
2:D:95:PRO:O	2:D:99:GLU:HG2	2.14	0.47
2:B:263:PHE:CE1	2:B:274:ILE:HG13	2.49	0.47
2:D:204:TYR:HB2	2:D:235:TYR:CD1	2.50	0.47
1:A:129:LEU:HD21	1:A:327:GLU:HG2	1.97	0.47
1:A:689:GLN:O	1:A:693:ILE:HG12	2.14	0.47
1:C:562:PHE:HZ	1:C:570:ASN:HD22	1.62	0.47
1:A:148:SER:O	1:A:152:GLU:HG2	2.15	0.47
1:C:602:ALA:HB1	1:C:759:ARG:HH12	1.79	0.47
1:C:793:LEU:HD12	1:C:794:PRO:HD2	1.96	0.47
1:C:25:MET:O	1:C:29:LYS:HG3	2.15	0.47
1:C:929:ILE:HB	1:C:995:ASP:OD2	2.15	0.47
1:A:386:SER:HB2	1:A:391:HIS:NE2	2.30	0.47
1:A:29:LYS:HE2	1:A:265:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:GLU:OE2	2:B:68:TYR:HE2	1.98	0.47
1:A:98:TRP:CE3	1:A:98:TRP:HA	2.50	0.47
1:A:836:LYS:HB2	1:A:839:ASN:HB3	1.96	0.47
1:A:763:ASP:O	1:A:766:LYS:HB2	2.14	0.47
1:A:768:SER:HA	1:A:815:LEU:HD23	1.97	0.47
2:D:51:ILE:O	2:D:54:ILE:HG22	2.15	0.47
2:B:160:SER:HB2	2:B:169:TYR:CE1	2.49	0.46
6:A:1105:CLR:H25	1:C:993:VAL:HG21	1.98	0.46
1:C:191:ARG:HE	1:C:239:SER:HA	1.81	0.46
1:C:666:MET:HE3	1:C:670:GLN:HB3	1.97	0.46
1:C:768:SER:HA	1:C:815:LEU:HD23	1.98	0.46
2:B:217:ARG:HH11	2:B:217:ARG:CG	2.25	0.46
2:D:26:GLY:HA2	2:D:27:ARG:HA	1.62	0.46
1:C:473:ILE:HD12	1:C:483:LEU:HD21	1.97	0.46
1:C:998:ARG:HE	1:C:1014:THR:HB	1.81	0.46
1:A:762:PHE:CE1	1:A:837:LEU:HD13	2.51	0.46
1:C:944:ASN:O	1:C:948:ILE:HG12	2.16	0.46
1:A:883:TRP:HA	1:A:904:ARG:NH1	2.30	0.46
1:A:860:PHE:CZ	6:A:1105:CLR:H191	2.50	0.46
2:D:133:LEU:H	2:D:133:LEU:HD12	1.80	0.46
1:A:936:SER:HB2	1:A:1003:ARG:HH21	1.81	0.46
1:C:148:SER:O	1:C:152:GLU:HG2	2.15	0.46
2:D:148:VAL:HG11	2:D:255:LEU:H	1.81	0.46
1:C:98:TRP:HA	1:C:98:TRP:CE3	2.50	0.46
1:A:118:PRO:HA	1:A:121:ASP:CB	2.46	0.46
1:C:883:TRP:HA	1:C:904:ARG:HH11	1.81	0.46
1:C:883:TRP:HA	1:C:904:ARG:NH1	2.31	0.46
2:D:167:TYR:C	2:D:169:TYR:N	2.70	0.46
1:C:915:PHE:O	1:C:919:ILE:HG12	2.16	0.46
2:B:277:LYS:HB3	2:B:279:TYR:CE1	2.51	0.46
1:A:104:CYS:SG	1:A:322:VAL:HG11	2.56	0.46
2:B:21:LYS:HG3	2:B:22:LYS:H	1.81	0.46
1:A:611:GLY:HA2	1:A:686:THR:H	1.81	0.46
1:A:998:ARG:HE	1:A:1014:THR:HB	1.81	0.46
1:A:385:TRP:HE3	1:A:580:GLY:HA2	1.81	0.46
1:A:191:ARG:HE	1:A:239:SER:HA	1.80	0.46
1:C:794:PRO:HG2	1:C:859:PHE:HE1	1.80	0.45
2:B:148:VAL:HG11	2:B:255:LEU:H	1.81	0.45
1:C:957:LEU:O	1:C:961:LEU:HD12	2.16	0.45
2:B:170:LYS:CB	2:B:174:PRO:HA	2.36	0.45
1:A:490:ASN:OD1	1:A:490:ASN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:TYR:CE2	2:B:258:LEU:HD11	2.51	0.45
1:A:182:ASP:N	1:A:182:ASP:OD1	2.49	0.45
1:C:660:GLY:HA2	1:C:663:LEU:HB2	1.98	0.45
2:B:177:ILE:HA	2:B:260:ALA:HA	1.99	0.45
1:A:883:TRP:HA	1:A:904:ARG:HH11	1.81	0.45
2:B:91:ARG:HD2	2:B:94:ASP:H	1.82	0.45
2:B:229:TYR:CD1	2:B:261:VAL:HG22	2.52	0.45
1:C:41:LEU:HD12	1:C:41:LEU:H	1.80	0.45
2:B:105:ILE:HG22	2:B:109:LEU:HD13	1.98	0.45
2:B:244:PRO:HG2	2:B:246:TYR:CE1	2.51	0.45
2:D:112:TYR:CE2	2:D:258:LEU:HD11	2.51	0.45
1:A:78:THR:OG1	1:A:80:PRO:HD3	2.16	0.45
9:B:1005:17F:H18A	9:B:1005:17F:H32	1.67	0.45
1:A:1009:TRP:HB3	10:A:1110:CE1:C24	2.44	0.45
1:A:901:TYR:HA	1:A:904:ARG:HE	1.81	0.45
1:C:708:THR:HG22	1:C:725:VAL:HB	1.98	0.45
1:C:773:LEU:HA	1:C:773:LEU:HD23	1.77	0.45
1:A:157:MET:HB3	1:A:157:MET:HE3	1.90	0.45
1:C:182:ASP:N	1:C:182:ASP:OD1	2.48	0.45
1:A:880:ARG:HH21	5:A:1104:OBN:C6'	2.29	0.45
1:C:710:ASP:O	1:C:731:GLY:HA2	2.17	0.45
1:A:872:LEU:HD13	1:A:872:LEU:HA	1.86	0.45
6:E:2001:CLR:H211	6:E:2001:CLR:H231	1.69	0.45
1:A:286:HIS:HB3	9:A:1109:17F:H1A	1.99	0.45
5:C:2004:OBN:O1	5:C:2004:OBN:O3	2.28	0.45
2:D:21:LYS:HG3	2:D:22:LYS:H	1.81	0.45
1:A:986:PRO:HG3	6:A:1105:CLR:H152	1.97	0.45
2:D:164:ASP:N	2:D:164:ASP:OD1	2.50	0.45
2:B:241:GLN:H	2:B:241:GLN:HG2	1.63	0.45
2:B:230:PHE:HD2	2:B:260:ALA:HB3	1.81	0.45
1:A:840:GLU:CD	1:A:840:GLU:H	2.19	0.45
2:B:164:ASP:N	2:B:164:ASP:OD1	2.50	0.45
1:A:786:PHE:CZ	5:A:1104:OBN:H6'1	2.52	0.45
1:C:862:TYR:C	1:C:862:TYR:CD1	2.90	0.44
1:A:862:TYR:C	1:A:862:TYR:CD1	2.90	0.44
7:A:1106:1AT:H18	2:D:68:TYR:OH	2.17	0.44
2:B:251:GLN:HB3	2:B:254:TYR:HB2	1.99	0.44
1:A:430:GLN:CG	1:A:438:ARG:HB2	2.47	0.44
2:D:108:PHE:HZ	2:D:179:LYS:HD3	1.82	0.44
2:B:133:LEU:HD12	2:B:133:LEU:H	1.81	0.44
1:A:340:THR:O	1:A:344:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:277:LYS:HB3	2:D:279:TYR:CE1	2.52	0.44
2:D:241:GLN:H	2:D:241:GLN:HG2	1.61	0.44
1:C:118:PRO:HA	1:C:121:ASP:CB	2.47	0.44
2:D:251:GLN:HB3	2:D:254:TYR:HB2	1.99	0.44
2:D:216:LYS:HE3	2:D:222:GLU:OE1	2.17	0.44
1:A:957:LEU:O	1:A:961:LEU:HD12	2.16	0.44
1:A:689:GLN:N	1:A:689:GLN:OE1	2.38	0.44
1:C:794:PRO:CB	1:C:862:TYR:CD2	3.00	0.44
1:A:793:LEU:HD12	1:A:794:PRO:HD2	1.99	0.44
1:A:880:ARG:HG3	1:A:881:VAL:N	2.33	0.44
1:C:385:TRP:HE3	1:C:580:GLY:HA2	1.81	0.44
1:A:473:ILE:HD12	1:A:483:LEU:HD21	1.99	0.44
1:C:490:ASN:OD1	1:C:490:ASN:N	2.48	0.44
1:C:280:GLU:OE2	1:C:830:ARG:NH2	2.51	0.44
2:B:167:TYR:C	2:B:169:TYR:N	2.69	0.44
2:D:71:ARG:HD3	2:D:71:ARG:HA	1.76	0.44
1:A:1009:TRP:H	10:A:1110:CE1:C26	2.30	0.44
2:D:221:LYS:HE3	2:D:223:LYS:HG3	2.00	0.44
8:A:1107:1DS:O4	2:B:68:TYR:OH	2.33	0.44
1:C:430:GLN:CG	1:C:438:ARG:HB2	2.47	0.44
1:C:762:PHE:CE1	1:C:837:LEU:HD13	2.53	0.44
1:A:729:ILE:HG13	1:A:730:ALA:N	2.33	0.44
1:A:424:ALA:O	1:A:464:ARG:NH2	2.50	0.44
2:D:80:ILE:HG12	2:D:177:ILE:HB	2.00	0.44
1:C:913:THR:N	1:C:914:PRO:HD2	2.33	0.44
1:C:78:THR:OG1	1:C:80:PRO:HD3	2.18	0.44
2:B:221:LYS:HE3	2:B:223:LYS:HG3	2.00	0.44
1:A:982:PHE:CD2	8:A:1107:1DS:H24	2.53	0.44
2:D:105:ILE:HG22	2:D:109:LEU:HD13	1.99	0.44
2:D:177:ILE:HA	2:D:260:ALA:HA	2.00	0.44
1:C:901:TYR:HA	1:C:904:ARG:HE	1.81	0.44
1:C:936:SER:HB2	1:C:1003:ARG:HH21	1.82	0.44
2:B:80:ILE:HG12	2:B:177:ILE:HB	2.00	0.43
1:C:116:GLU:HG3	1:C:118:PRO:CD	2.40	0.43
1:A:600:ARG:NH2	1:A:680:GLU:HG2	2.33	0.43
1:C:487:LYS:NZ	1:C:560:GLU:O	2.45	0.43
1:C:986:PRO:HB2	6:C:2005:CLR:H262	2.00	0.43
2:B:71:ARG:HA	2:B:71:ARG:HD3	1.77	0.43
1:C:840:GLU:CD	1:C:840:GLU:H	2.22	0.43
8:A:1107:1DS:O3'	8:A:1107:1DS:O6'	2.29	0.43
1:A:374:LEU:O	1:A:592:VAL:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:VAL:HG21	1:C:847:TYR:CE2	2.53	0.43
1:A:660:GLY:HA2	1:A:663:LEU:HB2	2.00	0.43
1:A:93:PHE:HA	1:A:285:ILE:HD11	2.01	0.43
1:A:229:PRO:O	1:A:232:THR:HG22	2.18	0.43
1:C:29:LYS:HE3	1:C:29:LYS:HB3	1.87	0.43
2:B:108:PHE:HZ	2:B:179:LYS:HD3	1.83	0.43
1:C:909:PHE:CE2	1:C:972:ARG:CZ	3.01	0.43
1:C:762:PHE:CE2	1:C:830:ARG:HD2	2.54	0.43
1:C:413:ALA:O	1:C:417:ILE:HG13	2.18	0.43
1:A:326:PRO:HA	13:A:1203:HOH:O	2.18	0.43
2:B:193:ASN:OD1	2:B:205:ASN:ND2	2.51	0.43
1:A:183:LEU:HD21	1:A:248:ARG:NH2	2.34	0.43
1:A:612:ASP:OD1	1:A:613:HIS:N	2.39	0.43
1:A:886:ARG:HA	1:A:901:TYR:CD1	2.54	0.43
1:C:503:ALA:HA	1:C:504:PRO:HD3	1.90	0.43
1:C:963:TYR:CD2	3:E:30:GLY:HA3	2.54	0.43
1:C:374:LEU:O	1:C:592:VAL:HG21	2.18	0.43
2:D:62:SER:HB3	2:D:65:LYS:O	2.19	0.43
1:C:324:ASN:O	1:C:326:PRO:HD3	2.18	0.43
1:A:758:GLY:HA2	1:A:761:ILE:HG22	2.01	0.43
1:A:225:THR:HG21	1:A:233:ARG:HD2	2.01	0.43
2:D:80:ILE:HG21	2:D:177:ILE:HD12	2.00	0.43
1:A:90:PHE:O	1:A:94:SER:HB2	2.19	0.43
1:C:90:PHE:O	1:C:94:SER:HB2	2.19	0.43
1:C:611:GLY:HA2	1:C:686:THR:H	1.83	0.43
1:C:183:LEU:HD21	1:C:248:ARG:NH2	2.34	0.43
2:D:91:ARG:HD2	2:D:94:ASP:H	1.82	0.43
1:C:340:THR:O	1:C:344:MET:HG2	2.18	0.43
1:A:831:ASN:HA	1:A:832:PRO:HD2	1.90	0.43
1:A:397:GLU:HG2	1:A:397:GLU:H	1.62	0.43
1:A:413:ALA:O	1:A:417:ILE:HG13	2.18	0.43
2:D:206:PRO:HB2	2:D:207:TYR:CD2	2.54	0.43
2:B:21:LYS:HA	2:B:21:LYS:HD2	1.58	0.43
1:C:743:LEU:HD11	1:C:751:ILE:HD13	2.00	0.43
10:E:2002:CE1:H122	10:E:2002:CE1:H151	1.73	0.43
2:B:288:LYS:HD2	2:B:288:LYS:HA	1.80	0.43
2:B:274:ILE:HD13	2:B:274:ILE:HA	1.78	0.43
2:D:187:LYS:O	2:D:282:ASN:ND2	2.52	0.43
1:A:435:ILE:O	1:A:438:ARG:HG2	2.19	0.43
1:C:964:CYS:HB3	1:C:967:MET:HG3	2.01	0.43
1:A:267:ALA:CB	1:A:715:SER:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ASP:HB2	1:A:243:VAL:CG2	2.48	0.43
1:A:762:PHE:CE2	1:A:830:ARG:HD2	2.54	0.43
1:C:424:ALA:O	1:C:464:ARG:NH2	2.51	0.43
2:D:217:ARG:HH11	2:D:217:ARG:CG	2.26	0.42
1:A:913:THR:N	1:A:914:PRO:HD2	2.33	0.42
1:A:212:THR:HG21	1:A:214:GLU:OE1	2.18	0.42
1:C:435:ILE:O	1:C:438:ARG:HG2	2.18	0.42
1:C:416:ARG:HD2	1:C:467:TYR:OH	2.19	0.42
1:A:56:LEU:HD11	1:A:182:ASP:HB3	2.01	0.42
1:A:295:LEU:HA	1:A:295:LEU:HD23	1.75	0.42
1:C:862:TYR:C	1:C:862:TYR:HD1	2.23	0.42
1:A:280:GLU:OE2	1:A:830:ARG:NH2	2.52	0.42
1:C:225:THR:HG21	1:C:233:ARG:HD2	2.01	0.42
1:A:205:LYS:HA	1:A:219:THR:HA	2.01	0.42
10:A:1110:CE1:H212	10:A:1110:CE1:C27	2.44	0.42
1:C:880:ARG:HG3	1:C:881:VAL:N	2.33	0.42
1:A:803:ILE:HD13	1:A:803:ILE:HA	1.85	0.42
1:C:860:PHE:O	1:C:864:VAL:HG23	2.19	0.42
1:A:843:ILE:HB	9:A:1108:17F:H5	2.02	0.42
6:G:1001:CLR:H211	6:G:1001:CLR:H231	1.70	0.42
1:C:936:SER:OG	1:C:996:GLU:OE2	2.28	0.42
1:C:207:ASP:HB2	1:C:243:VAL:CG2	2.49	0.42
1:A:54:ARG:HB3	1:A:54:ARG:HE	1.54	0.42
2:D:231:GLY:HA3	2:D:235:TYR:O	2.19	0.42
1:C:907:VAL:O	1:C:911:CYS:HB2	2.20	0.42
2:B:117:GLN:HA	2:B:123:PHE:CE2	2.54	0.42
1:C:420:LEU:HB3	1:C:486:HIS:HE1	1.83	0.42
1:A:416:ARG:HD2	1:A:467:TYR:OH	2.19	0.42
1:A:254:THR:O	1:A:257:ARG:NE	2.49	0.42
2:D:274:ILE:HA	2:D:274:ILE:HD13	1.78	0.42
1:C:898:GLN:HE22	2:D:179:LYS:HE3	1.84	0.42
1:A:890:ASP:OD1	2:B:82:GLN:NE2	2.53	0.42
1:A:773:LEU:HD23	1:A:773:LEU:HA	1.78	0.42
1:A:470:ILE:HD12	1:A:564:PHE:CE1	2.54	0.42
1:C:462:GLU:HA	1:C:465:GLU:HG2	2.02	0.42
1:C:729:ILE:HG13	1:C:730:ALA:N	2.34	0.42
1:C:866:LEU:HA	1:C:866:LEU:HD23	1.65	0.42
2:B:204:TYR:HB2	2:B:235:TYR:CD1	2.54	0.42
2:D:24:PHE:CD1	2:D:28:THR:HG22	2.54	0.42
1:A:479:ASN:OD1	1:A:506:ARG:NH1	2.53	0.42
2:B:174:PRO:O	2:B:263:PHE:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:117:GLN:HA	2:D:123:PHE:CE2	2.54	0.42
2:B:91:ARG:H	2:B:97:SER:HG	1.65	0.42
1:A:76:PRO:HA	1:A:77:PRO:HD3	1.85	0.42
2:B:178:ILE:HD12	2:B:211:VAL:HG11	2.01	0.42
1:C:194:ALA:HB1	1:C:253:TYR:O	2.20	0.42
1:A:710:ASP:O	1:A:731:GLY:HA2	2.20	0.42
2:D:244:PRO:HG2	2:D:246:TYR:HE1	1.84	0.42
1:C:600:ARG:NH2	1:C:680:GLU:HG2	2.34	0.42
1:A:462:GLU:HA	1:A:465:GLU:HG2	2.02	0.42
2:D:229:TYR:CD1	2:D:261:VAL:HG22	2.54	0.42
1:A:103:LEU:HB3	1:A:318:ILE:HG23	2.01	0.42
1:A:504:PRO:HG2	1:A:535:TYR:CE1	2.55	0.42
2:B:231:GLY:HA3	2:B:235:TYR:O	2.20	0.42
3:E:42:LEU:HA	3:E:45:ILE:HD11	2.01	0.42
1:C:880:ARG:NH2	5:C:2004:OBN:H6'2	2.35	0.42
1:C:467:TYR:HB3	1:C:486:HIS:HB3	2.02	0.42
1:A:467:TYR:HB3	1:A:486:HIS:HB3	2.02	0.42
1:A:964:CYS:HB3	1:A:967:MET:HG3	2.01	0.42
2:B:139:TYR:OH	2:B:185:GLY:HA2	2.20	0.42
1:C:982:PHE:CE1	6:E:2001:CLR:H183	2.55	0.41
2:D:204:TYR:O	2:D:208:VAL:CG1	2.61	0.41
1:C:886:ARG:HA	1:C:901:TYR:CD1	2.55	0.41
1:C:480:LYS:HE3	1:C:506:ARG:HH11	1.85	0.41
1:A:42:ASP:O	1:A:46:ARG:HB2	2.19	0.41
1:C:205:LYS:HA	1:C:219:THR:HA	2.02	0.41
2:D:139:TYR:OH	2:D:185:GLY:HA2	2.20	0.41
1:A:1002:ILE:HD13	1:A:1015:TYR:HB2	2.01	0.41
2:B:80:ILE:HG21	2:B:177:ILE:HD12	2.00	0.41
10:A:1110:CE1:H212	10:A:1110:CE1:H242	1.66	0.41
2:D:167:TYR:O	2:D:167:TYR:CG	2.73	0.41
6:A:1105:CLR:H162	6:A:1105:CLR:H241	2.01	0.41
1:C:97:LEU:HB2	1:C:133:VAL:HG22	2.02	0.41
1:C:56:LEU:HD11	1:C:182:ASP:HB3	2.01	0.41
10:A:1110:CE1:H101	2:B:38:PHE:HA	2.02	0.41
1:C:212:THR:HG21	1:C:214:GLU:OE1	2.20	0.41
1:A:469:LYS:HB2	1:A:469:LYS:HE3	1.82	0.41
1:A:982:PHE:CE1	6:G:1001:CLR:H183	2.54	0.41
1:C:208:ASN:HB3	1:C:212:THR:CG2	2.49	0.41
1:A:420:LEU:HB3	1:A:486:HIS:HE1	1.84	0.41
1:C:192:ILE:HB	1:C:237:PHE:O	2.19	0.41
1:C:872:LEU:HD13	1:C:872:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:963:TYR:HE2	6:G:1001:CLR:H6	1.83	0.41
1:A:194:ALA:HB1	1:A:253:TYR:O	2.20	0.41
1:C:462:GLU:O	1:C:466:ARG:HB2	2.21	0.41
2:D:83:SER:OG	2:D:87:GLU:O	2.33	0.41
1:A:862:TYR:C	1:A:862:TYR:HD1	2.23	0.41
1:C:977:LYS:HE2	2:D:68:TYR:CD1	2.55	0.41
1:A:783:PHE:CD2	5:A:1104:OBN:H161	2.55	0.41
3:G:42:LEU:HA	3:G:45:ILE:HD11	2.03	0.41
2:B:187:LYS:O	2:B:282:ASN:ND2	2.54	0.41
2:B:244:PRO:HG2	2:B:246:TYR:HE1	1.85	0.41
1:A:324:ASN:O	1:A:326:PRO:HD3	2.21	0.41
1:A:803:ILE:HG12	1:A:916:PHE:HD1	1.85	0.41
1:A:921:VAL:HG13	1:A:924:TRP:CZ3	2.56	0.41
2:B:166:THR:HG21	2:B:170:LYS:H	1.86	0.41
1:C:963:TYR:HE2	6:E:2001:CLR:H6	1.84	0.41
2:B:216:LYS:HE3	2:B:222:GLU:OE1	2.20	0.41
1:A:207:ASP:OD1	1:A:209:SER:HB3	2.21	0.41
1:C:82:TRP:CD1	1:C:141:TYR:OH	2.74	0.41
2:B:226:THR:HB	2:B:265:ASN:HB2	2.03	0.41
1:C:921:VAL:HG13	1:C:924:TRP:CZ3	2.56	0.41
1:C:783:PHE:CD2	5:C:2004:OBN:H161	2.55	0.41
2:D:22:LYS:HA	2:D:23:GLU:HA	1.77	0.41
1:A:614:PRO:HD3	1:A:685:ARG:HD2	2.02	0.41
1:C:504:PRO:HG2	1:C:535:TYR:CE1	2.56	0.41
1:C:216:GLU:HG2	1:C:216:GLU:H	1.64	0.41
2:D:111:LYS:H	2:D:111:LYS:HG3	1.71	0.41
1:C:803:ILE:HG12	1:C:916:PHE:HD1	1.86	0.41
1:C:1002:ILE:HD13	1:C:1015:TYR:HB2	2.01	0.41
2:D:174:PRO:O	2:D:263:PHE:N	2.46	0.41
2:B:204:TYR:CA	2:B:206:PRO:HD2	2.50	0.41
1:A:963:TYR:CD2	3:G:30:GLY:HA3	2.56	0.41
2:D:160:SER:HB2	2:D:169:TYR:CE1	2.55	0.41
1:A:907:VAL:O	1:A:911:CYS:HB2	2.21	0.41
3:G:33:PHE:HA	9:G:1002:17F:C18	2.51	0.41
1:C:506:ARG:O	1:C:509:ASP:HB3	2.21	0.41
1:A:97:LEU:HB2	1:A:133:VAL:HG22	2.03	0.41
1:A:462:GLU:O	1:A:466:ARG:HB2	2.21	0.41
1:C:61:ALA:O	1:C:179:VAL:HG11	2.20	0.41
2:D:80:ILE:CD1	2:D:177:ILE:H	2.34	0.41
1:C:93:PHE:HA	1:C:285:ILE:HD11	2.02	0.41
1:A:1005:ARG:HH21	10:A:1110:CE1:H291	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LEU:CD2	1:A:572:PRO:HG2	2.51	0.40
1:C:416:ARG:NH1	1:C:467:TYR:OH	2.37	0.40
1:C:493:GLU:H	1:C:493:GLU:HG2	1.70	0.40
1:C:267:ALA:CB	1:C:715:SER:HB3	2.51	0.40
1:C:229:PRO:O	1:C:232:THR:HG22	2.20	0.40
2:D:37:LEU:O	2:D:41:ILE:HG12	2.21	0.40
1:A:82:TRP:CD1	1:A:141:TYR:OH	2.73	0.40
1:A:794:PRO:O	1:A:912:HIS:HD2	2.04	0.40
2:B:170:LYS:HD3	2:B:175:CYS:H	1.85	0.40
2:D:217:ARG:HG2	2:D:217:ARG:NH1	2.28	0.40
1:C:129:LEU:CD2	1:C:327:GLU:HG2	2.51	0.40
1:A:61:ALA:O	1:A:179:VAL:HG11	2.21	0.40
1:C:826:LYS:HD2	1:C:826:LYS:HA	1.82	0.40
2:B:17:TRP:CE3	2:B:17:TRP:HA	2.55	0.40
1:C:758:GLY:HA2	1:C:761:ILE:HG22	2.02	0.40
2:B:167:TYR:O	2:B:167:TYR:CG	2.73	0.40
2:B:80:ILE:HG23	2:B:177:ILE:HB	2.04	0.40
1:A:840:GLU:CD	9:A:1108:17F:N1	2.75	0.40
1:A:689:GLN:O	1:A:692:LEU:HB3	2.22	0.40
2:D:202:MET:CE	2:D:202:MET:HA	2.51	0.40
5:A:1104:OBN:H191	5:A:1104:OBN:H8	1.94	0.40
1:A:308:TYR:HE1	1:A:880:ARG:HH12	1.70	0.40
1:A:810:VAL:HB	1:A:811:PRO:HD3	2.03	0.40
1:C:918:THR:O	1:C:922:VAL:HG22	2.21	0.40
1:A:649:ASN:HA	1:A:650:PRO:HD3	1.89	0.40
2:D:170:LYS:HD3	2:D:175:CYS:H	1.86	0.40
2:B:80:ILE:HG12	2:B:177:ILE:N	2.36	0.40
2:D:204:TYR:HD2	2:D:235:TYR:CE1	2.39	0.40
1:A:108:TYR:HB2	1:A:122:ASN:HB3	2.03	0.40
1:C:493:GLU:O	1:C:493:GLU:HG2	2.22	0.40
1:C:157:MET:HE3	1:C:157:MET:HB3	1.97	0.40
1:C:801:LEU:HA	1:C:801:LEU:HD23	1.73	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	993/1021 (97%)	940 (95%)	51 (5%)	2 (0%)	52 87
1	C	993/1021 (97%)	947 (95%)	44 (4%)	2 (0%)	52 87
2	B	287/303 (95%)	255 (89%)	28 (10%)	4 (1%)	14 55
2	D	285/303 (94%)	255 (90%)	26 (9%)	4 (1%)	14 55
3	E	30/65 (46%)	28 (93%)	2 (7%)	0	100 100
3	G	30/65 (46%)	28 (93%)	2 (7%)	0	100 100
All	All	2618/2778 (94%)	2453 (94%)	153 (6%)	12 (0%)	34 75

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	199	TYR
2	D	199	TYR
2	B	161	GLY
2	D	161	GLY
2	B	170	LYS
2	B	196	LEU
2	D	170	LYS
2	D	196	LEU
1	A	118	PRO
1	C	118	PRO
1	A	489	PRO
1	C	489	PRO

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	846/864 (98%)	777 (92%)	69 (8%)	14 50
1	C	846/864 (98%)	780 (92%)	66 (8%)	16 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	259/269 (96%)	225 (87%)	34 (13%)	5 25
2	D	257/269 (96%)	226 (88%)	31 (12%)	6 28
3	E	26/52 (50%)	23 (88%)	3 (12%)	7 31
3	G	26/52 (50%)	23 (88%)	3 (12%)	7 31
All	All	2260/2370 (95%)	2054 (91%)	206 (9%)	12 44

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	25	MET
1	A	26	ASP
1	A	34	MET
1	A	35	ASP
1	A	45	HIS
1	A	53	SER
1	A	56	LEU
1	A	85	PHE
1	A	86	CYS
1	A	93	PHE
1	A	98	TRP
1	A	99	ILE
1	A	114	THR
1	A	117	GLU
1	A	120	ASN
1	A	121	ASP
1	A	123	LEU
1	A	124	TYR
1	A	127	VAL
1	A	150	ILE
1	A	157	MET
1	A	170	LYS
1	A	172	SER
1	A	180	VAL
1	A	209	SER
1	A	219	THR
1	A	220	ARG
1	A	231	GLU
1	A	238	PHE
1	A	275	THR
1	A	301	ILE

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Mol	Chain	Res	Type
1	A	314	VAL
1	A	324	ASN
1	A	327	GLU
1	A	350	LEU
1	A	357	VAL
1	A	420	LEU
1	A	431	GLU
1	A	433	LEU
1	A	459	SER
1	A	488	ASN
1	A	490	ASN
1	A	495	ARG
1	A	531	PHE
1	A	552	PHE
1	A	564	PHE
1	A	565	ASP
1	A	567	ASP
1	A	643	ILE
1	A	663	LEU
1	A	685	ARG
1	A	746	ASP
1	A	748	PHE
1	A	750	SER
1	A	762	PHE
1	A	815	LEU
1	A	824	ILE
1	A	840	GLU
1	A	862	TYR
1	A	880	ARG
1	A	904	ARG
1	A	911	CYS
1	A	928	VAL
1	A	957	LEU
1	A	961	LEU
1	A	979	THR
1	A	980	TRP
1	A	1000	LEU
2	B	15	PHE
2	B	17	TRP
2	B	19	SER
2	B	22	LYS
2	B	28	THR

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Mol	Chain	Res	Type
2	B	37	LEU
2	B	54	ILE
2	B	56	VAL
2	B	60	THR
2	B	79	GLN
2	B	80	ILE
2	B	105	ILE
2	B	119	ASP
2	B	156	LEU
2	B	159	CYS
2	B	162	LEU
2	B	164	ASP
2	B	167	TYR
2	B	169	TYR
2	B	170	LYS
2	B	171	ASP
2	B	178	ILE
2	B	195	SER
2	B	202	MET
2	B	203	LYS
2	B	204	TYR
2	B	217	ARG
2	B	223	LYS
2	B	224	VAL
2	B	259	MET
2	B	270	THR
2	B	274	ILE
2	B	282	ASN
2	B	287	GLU
3	G	32	ILE
3	G	45	ILE
3	G	47	SER
1	C	22	GLU
1	C	25	MET
1	C	26	ASP
1	C	34	MET
1	C	35	ASP
1	C	45	HIS
1	C	46	ARG
1	C	53	SER
1	C	56	LEU
1	C	85	PHE

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Mol	Chain	Res	Type
1	C	86	CYS
1	C	93	PHE
1	C	98	TRP
1	C	99	ILE
1	C	114	THR
1	C	117	GLU
1	C	120	ASN
1	C	121	ASP
1	C	123	LEU
1	C	124	TYR
1	C	127	VAL
1	C	150	ILE
1	C	157	MET
1	C	170	LYS
1	C	172	SER
1	C	180	VAL
1	C	209	SER
1	C	219	THR
1	C	220	ARG
1	C	231	GLU
1	C	238	PHE
1	C	275	THR
1	C	314	VAL
1	C	324	ASN
1	C	327	GLU
1	C	350	LEU
1	C	357	VAL
1	C	420	LEU
1	C	431	GLU
1	C	433	LEU
1	C	459	SER
1	C	488	ASN
1	C	490	ASN
1	C	495	ARG
1	C	531	PHE
1	C	552	PHE
1	C	643	ILE
1	C	663	LEU
1	C	685	ARG
1	C	746	ASP
1	C	748	PHE
1	C	750	SER

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Mol	Chain	Res	Type
1	C	762	PHE
1	C	815	LEU
1	C	824	ILE
1	C	840	GLU
1	C	862	TYR
1	C	880	ARG
1	C	904	ARG
1	C	911	CYS
1	C	928	VAL
1	C	957	LEU
1	C	961	LEU
1	C	979	THR
1	C	980	TRP
1	C	1000	LEU
2	D	17	TRP
2	D	19	SER
2	D	22	LYS
2	D	28	THR
2	D	54	ILE
2	D	56	VAL
2	D	60	THR
2	D	79	GLN
2	D	80	ILE
2	D	105	ILE
2	D	119	ASP
2	D	156	LEU
2	D	159	CYS
2	D	164	ASP
2	D	167	TYR
2	D	169	TYR
2	D	170	LYS
2	D	171	ASP
2	D	178	ILE
2	D	195	SER
2	D	202	MET
2	D	203	LYS
2	D	204	TYR
2	D	217	ARG
2	D	223	LYS
2	D	224	VAL
2	D	259	MET
2	D	270	THR

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Mol	Chain	Res	Type
2	D	274	ILE
2	D	282	ASN
2	D	287	GLU
3	E	32	ILE
3	E	45	ILE
3	E	47	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	HIS
2	B	241	GLN
1	C	486	HIS
2	D	241	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PHD	A	369	1,4	8,11,12	1.13	1 (12%)	9,15,17	1.65	3 (33%)
1	PHD	C	369	1,4	8,11,12	1.12	1 (12%)	9,15,17	1.61	3 (33%)

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
1	PHD	A	369	1,4	-	0/7/11/13	0/0/0/0
1	PHD	C	369	1,4	-	0/7/11/13	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	369	PHD	CB-CA	-2.21	1.49	1.53
1	A	369	PHD	CB-CA	-2.08	1.49	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	369	PHD	OD2-CG-CB	-2.83	118.19	124.69
1	C	369	PHD	OD2-CG-CB	-2.58	118.77	124.69
1	A	369	PHD	O-C-CA	-2.53	118.91	125.49
1	C	369	PHD	O-C-CA	-2.43	119.16	125.49
1	C	369	PHD	CA-CB-CG	2.19	116.86	113.06
1	A	369	PHD	CA-CB-CG	2.34	117.11	113.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

2 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	NAG	B	1001	11,2	14,14,15	0.33	0	15,19,21	0.38	0
11	NAG	B	1002	11	14,14,15	0.23	0	15,19,21	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	B	1001	11,2	-	0/6/23/26	0/1/1/1
11	NAG	B	1002	11	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
5	OBN	A	1104	-	44,46,46	0.79	1 (2%)	65,76,76	1.80	15 (23%)
6	CLR	A	1105	-	31,31,31	2.29	7 (22%)	48,48,48	2.63	16 (33%)
7	1AT	A	1106	-	30,30,35	1.41	3 (10%)	43,43,48	2.38	15 (34%)
8	1DS	A	1107	-	30,30,35	1.26	4 (13%)	42,43,48	2.23	15 (35%)
9	17F	A	1108	-	14,17,53	1.35	2 (14%)	13,23,60	3.29	4 (30%)
9	17F	A	1109	-	14,17,53	1.21	2 (14%)	13,23,60	3.46	6 (46%)
10	CE1	A	1110	-	33,33,36	0.57	0	32,32,35	0.95	1 (3%)
12	NAG	B	1003	2	14,14,15	0.31	0	15,19,21	0.47	0
12	NAG	B	1004	2	14,14,15	0.47	0	15,19,21	0.23	0
9	17F	B	1005	-	20,23,53	1.21	2 (10%)	20,29,60	3.01	7 (35%)
5	OBN	C	2004	-	44,46,46	0.74	1 (2%)	65,76,76	1.70	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CLR	C	2005	-	31,31,31	2.26	8 (25%)	48,48,48	2.61	17 (35%)
12	NAG	D	2001	2	14,14,15	0.34	0	15,19,21	0.38	0
12	NAG	D	2002	2	14,14,15	0.58	0	15,19,21	0.53	0
12	NAG	D	2003	2	14,14,15	0.54	0	15,19,21	0.49	0
9	17F	D	2004	-	24,27,53	1.10	3 (12%)	24,34,60	2.03	7 (29%)
6	CLR	E	2001	-	31,31,31	2.23	8 (25%)	48,48,48	2.52	17 (35%)
10	CE1	E	2002	-	21,21,36	0.71	0	20,20,35	1.18	3 (15%)
6	CLR	G	1001	-	31,31,31	2.25	8 (25%)	48,48,48	2.52	17 (35%)
9	17F	G	1002	-	23,26,53	1.11	2 (8%)	23,33,60	2.94	7 (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
5	OBN	A	1104	-	-	0/11/116/116	0/6/6/6
6	CLR	A	1105	-	-	0/10/68/68	0/4/4/4
7	1AT	A	1106	-	-	0/19/58/63	0/2/2/2
8	1DS	A	1107	-	-	0/19/58/63	0/2/2/2
9	17F	A	1108	-	-	0/16/20/59	0/0/0/0
9	17F	A	1109	-	-	1/16/20/59	0/0/0/0
10	CE1	A	1110	-	-	0/31/31/34	0/0/0/0
12	NAG	B	1003	2	-	0/6/23/26	0/1/1/1
12	NAG	B	1004	2	-	0/6/23/26	0/1/1/1
9	17F	B	1005	-	-	0/23/27/59	0/0/0/0
5	OBN	C	2004	-	-	0/11/116/116	0/6/6/6
6	CLR	C	2005	-	-	0/10/68/68	0/4/4/4
12	NAG	D	2001	2	-	0/6/23/26	0/1/1/1
12	NAG	D	2002	2	-	0/6/23/26	0/1/1/1
12	NAG	D	2003	2	-	0/6/23/26	0/1/1/1
9	17F	D	2004	-	-	0/29/33/59	0/0/0/0
6	CLR	E	2001	-	-	0/10/68/68	0/4/4/4
10	CE1	E	2002	-	-	0/19/19/34	0/0/0/0
6	CLR	G	1001	-	-	0/10/68/68	0/4/4/4
9	17F	G	1002	-	-	0/27/31/59	0/0/0/0

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	1002	17F	O9-C5	-3.32	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1005	17F	O9-C5	-3.27	1.41	1.47
9	A	1108	17F	O9-C5	-2.98	1.41	1.47
6	E	2001	CLR	C20-C17	-2.92	1.48	1.54
6	G	1001	CLR	C20-C17	-2.88	1.49	1.54
9	D	2004	17F	O7-C6	-2.85	1.38	1.45
6	E	2001	CLR	C13-C17	-2.84	1.49	1.55
6	G	1001	CLR	C13-C17	-2.84	1.49	1.55
8	A	1107	1DS	C1'-C2'	-2.77	1.48	1.52
6	E	2001	CLR	C15-C14	-2.59	1.48	1.54
9	A	1109	17F	O9-C5	-2.51	1.42	1.47
7	A	1106	1AT	C4'-C5'	-2.50	1.46	1.53
6	A	1105	CLR	C15-C14	-2.42	1.48	1.54
7	A	1106	1AT	C4-C5	-2.40	1.48	1.53
6	G	1001	CLR	C15-C14	-2.39	1.48	1.54
6	C	2005	CLR	C15-C14	-2.22	1.49	1.54
6	C	2005	CLR	C20-C17	-2.17	1.50	1.54
8	A	1107	1DS	C4'-C3'	-2.15	1.42	1.52
6	A	1105	CLR	C20-C17	-2.12	1.50	1.54
6	C	2005	CLR	C13-C17	-2.02	1.50	1.55
6	E	2001	CLR	C16-C17	2.02	1.59	1.54
9	D	2004	17F	O7-C7	2.03	1.39	1.33
6	C	2005	CLR	C16-C17	2.04	1.59	1.54
6	G	1001	CLR	C16-C17	2.07	1.59	1.54
9	D	2004	17F	O9-C17	2.30	1.41	1.34
6	A	1105	CLR	C16-C17	2.31	1.59	1.54
9	G	1002	17F	O7-C7	2.35	1.40	1.33
8	A	1107	1DS	C2N-C1N	2.38	1.57	1.50
8	A	1107	1DS	O1'-C1N	2.82	1.41	1.33
9	A	1109	17F	O9-C17	2.92	1.42	1.35
9	B	1005	17F	O9-C17	2.93	1.43	1.34
6	E	2001	CLR	C12-C13	2.99	1.59	1.54
6	G	1001	CLR	C12-C13	3.12	1.60	1.54
9	A	1108	17F	O9-C17	3.21	1.42	1.35
6	C	2005	CLR	C12-C13	3.26	1.60	1.54
5	C	2004	OBN	O21-C23	3.27	1.45	1.36
5	A	1104	OBN	O21-C23	3.28	1.45	1.36
6	A	1105	CLR	C12-C13	3.33	1.60	1.54
6	E	2001	CLR	C8-C14	3.51	1.60	1.53
6	G	1001	CLR	C8-C14	3.77	1.61	1.53
6	A	1105	CLR	C8-C14	3.83	1.61	1.53
6	C	2005	CLR	C8-C14	4.09	1.61	1.53
7	A	1106	1AT	O6-C1N	4.20	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	1001	CLR	C11-C9	4.23	1.61	1.53
6	E	2001	CLR	C11-C9	4.38	1.61	1.53
6	C	2005	CLR	C11-C9	4.73	1.62	1.53
6	A	1105	CLR	C11-C9	4.96	1.62	1.53
6	E	2001	CLR	C6-C5	8.17	1.53	1.33
6	G	1001	CLR	C6-C5	8.21	1.53	1.33
6	A	1105	CLR	C6-C5	8.36	1.53	1.33
6	C	2005	CLR	C6-C5	8.39	1.53	1.33

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1105	CLR	C4-C5-C6	-7.02	108.65	120.57
7	A	1106	1AT	O2-C2-C3	-7.00	94.58	110.34
6	A	1105	CLR	C7-C6-C5	-6.52	110.99	125.01
6	G	1001	CLR	C7-C6-C5	-6.26	111.56	125.01
6	E	2001	CLR	C7-C6-C5	-6.14	111.82	125.01
6	C	2005	CLR	C7-C6-C5	-6.03	112.05	125.01
6	G	1001	CLR	C4-C5-C6	-6.01	110.37	120.57
6	C	2005	CLR	C4-C5-C6	-5.92	110.53	120.57
6	E	2001	CLR	C4-C5-C6	-5.80	110.72	120.57
6	A	1105	CLR	C12-C13-C17	-5.77	106.31	116.56
5	A	1104	OBN	C6'-C5'-C4'	-5.73	101.79	113.08
6	E	2001	CLR	C12-C13-C17	-5.66	106.51	116.56
6	G	1001	CLR	C12-C13-C17	-5.60	106.61	116.56
6	E	2001	CLR	C10-C5-C6	-5.00	113.67	122.92
6	C	2005	CLR	C12-C13-C17	-4.91	107.83	116.56
6	C	2005	CLR	C10-C5-C6	-4.88	113.91	122.92
6	G	1001	CLR	C10-C5-C6	-4.57	114.47	122.92
6	A	1105	CLR	C19-C10-C9	-4.54	105.86	111.67
6	G	1001	CLR	C19-C10-C9	-4.35	106.10	111.67
6	A	1105	CLR	C10-C5-C6	-4.30	114.98	122.92
6	A	1105	CLR	C19-C10-C1	-4.24	103.08	109.43
6	E	2001	CLR	C19-C10-C9	-4.06	106.48	111.67
5	C	2004	OBN	C6-C5-C4	-3.99	107.20	111.18
5	A	1104	OBN	C5-C4-C3	-3.83	110.65	114.14
6	C	2005	CLR	C19-C10-C1	-3.79	103.74	109.43
5	A	1104	OBN	C6-C5-C4	-3.67	107.52	111.18
9	G	1002	17F	O9-C17-O10	-3.54	115.85	122.92
7	A	1106	1AT	C1'-C2'-C3'	-3.39	103.04	114.49
8	A	1107	1DS	O2'-C2'-C3'	-3.34	97.97	105.58
9	A	1108	17F	O10-C17-C18	-3.24	112.86	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	2005	CLR	C21-C20-C22	-3.24	104.95	110.35
9	A	1109	17F	O10-C17-C18	-3.16	113.16	124.85
5	C	2004	OBN	C5-C4-C3	-3.16	111.27	114.14
8	A	1107	1DS	O3'-C3'-C4'	-3.14	102.00	113.29
9	D	2004	17F	O10-C17-C18	-3.14	111.16	123.72
8	A	1107	1DS	C1-C2-C3	-2.96	104.14	109.97
6	E	2001	CLR	C21-C20-C22	-2.95	105.44	110.35
5	A	1104	OBN	C6-C7-C8	-2.92	108.18	113.10
5	C	2004	OBN	C17-C20-C22	-2.80	121.03	128.64
5	A	1104	OBN	C17-C20-C22	-2.73	121.23	128.64
6	G	1001	CLR	C21-C20-C22	-2.71	105.83	110.35
6	E	2001	CLR	C16-C17-C13	-2.68	100.33	103.82
5	C	2004	OBN	C7-C6-C5	-2.68	109.38	112.60
5	A	1104	OBN	C7-C6-C5	-2.67	109.39	112.60
5	A	1104	OBN	C18-C13-C12	-2.66	107.45	111.14
9	G	1002	17F	O9-C5-C6	-2.61	99.15	108.36
5	C	2004	OBN	C6-C7-C8	-2.61	108.70	113.10
9	D	2004	17F	O7-C7-O8	-2.56	116.89	123.49
6	E	2001	CLR	C11-C12-C13	-2.56	108.27	112.84
7	A	1106	1AT	O1N-C1N-C2N	-2.55	113.53	123.72
6	G	1001	CLR	C16-C17-C13	-2.47	100.61	103.82
5	C	2004	OBN	C18-C13-C12	-2.45	107.74	111.14
6	G	1001	CLR	C11-C12-C13	-2.40	108.56	112.84
6	C	2005	CLR	C19-C10-C9	-2.38	108.62	111.67
8	A	1107	1DS	O1-C2'-C1'	-2.34	102.10	109.85
5	C	2004	OBN	C6'-C5'-C4'	-2.33	108.49	113.08
7	A	1106	1AT	O1-C2'-O2'	-2.30	103.21	110.52
6	E	2001	CLR	C19-C10-C1	-2.21	106.12	109.43
7	A	1106	1AT	C1-O5-C5	-2.20	109.47	113.75
6	G	1001	CLR	C19-C10-C1	-2.16	106.19	109.43
6	E	2001	CLR	C4-C5-C10	-2.10	113.37	116.43
7	A	1106	1AT	O6'-C6'-C5'	-2.08	104.45	111.33
9	B	1005	17F	C6-C5-C4	-2.05	106.19	112.70
6	E	2001	CLR	C11-C9-C8	2.07	114.75	111.74
10	E	2002	CE1	O13-C12-C11	2.10	118.27	109.87
6	A	1105	CLR	C18-C13-C17	2.14	115.94	111.75
9	D	2004	17F	O7-C6-C5	2.17	114.54	108.69
6	C	2005	CLR	C2-C1-C10	2.17	117.36	112.75
9	B	1005	17F	O9-C5-C6	2.19	112.83	107.88
6	C	2005	CLR	C15-C14-C8	2.22	122.53	119.03
8	A	1107	1DS	O2'-C2'-C1'	2.22	112.71	107.59
6	G	1001	CLR	C11-C9-C8	2.23	114.99	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	2002	CE1	C20-O19-C18	2.25	122.99	113.31
6	C	2005	CLR	C12-C11-C9	2.28	116.94	113.10
6	A	1105	CLR	C17-C13-C14	2.29	102.79	100.09
6	A	1105	CLR	C12-C11-C9	2.32	117.02	113.10
6	G	1001	CLR	C1-C2-C3	2.33	114.21	110.43
9	D	2004	17F	C6-O7-C7	2.33	123.37	116.85
6	A	1105	CLR	C2-C3-C4	2.34	114.49	110.32
6	A	1105	CLR	C11-C9-C10	2.38	116.27	113.11
9	A	1109	17F	O9-C5-C6	2.39	113.27	107.88
9	B	1005	17F	C19-C18-C17	2.39	123.00	113.59
7	A	1106	1AT	C2'-C3'-C4'	2.40	108.04	102.00
8	A	1107	1DS	O5-C1-O1	2.42	118.09	109.96
6	A	1105	CLR	C3-C4-C5	2.43	116.83	111.82
10	A	1110	CE1	C20-O19-C18	2.44	123.78	113.31
7	A	1106	1AT	C6-O6-C1N	2.47	123.75	116.85
5	A	1104	OBN	O11-C11-C9	2.47	116.23	110.91
8	A	1107	1DS	O4-C4-C5	2.49	115.85	109.24
10	E	2002	CE1	C17-O16-C15	2.49	124.03	113.31
6	G	1001	CLR	C2-C1-C10	2.49	118.04	112.75
9	D	2004	17F	O7-C7-C8	2.50	119.50	111.90
5	A	1104	OBN	C14-C8-C9	2.51	117.59	113.03
6	E	2001	CLR	C2-C1-C10	2.53	118.11	112.75
8	A	1107	1DS	O2'-C5'-C6'	2.53	116.22	108.57
5	A	1104	OBN	C16-C17-C13	2.57	108.06	105.02
9	G	1002	17F	O7-C7-C8	2.59	119.79	111.90
5	C	2004	OBN	O11-C11-C9	2.65	116.61	110.91
6	C	2005	CLR	C22-C20-C17	2.66	115.83	110.24
5	C	2004	OBN	C14-C8-C9	2.68	117.90	113.03
5	C	2004	OBN	C15-C14-C13	2.70	105.49	103.35
8	A	1107	1DS	C2'-C3'-C4'	2.74	108.89	102.00
5	C	2004	OBN	C16-C17-C13	2.75	108.27	105.02
7	A	1106	1AT	O4'-C4'-C3'	2.85	121.08	112.01
7	A	1106	1AT	O2'-C2'-C1'	2.93	115.95	107.98
6	A	1105	CLR	C21-C20-C17	2.96	117.89	112.96
5	A	1104	OBN	O5'-C5'-C6'	2.97	113.12	106.64
6	C	2005	CLR	C21-C20-C17	2.99	117.94	112.96
9	G	1002	17F	O9-C17-C18	3.00	116.75	111.10
5	A	1104	OBN	C1'-O3-C3	3.00	121.78	115.01
5	A	1104	OBN	C15-C14-C13	3.02	105.74	103.35
8	A	1107	1DS	O3-C3-C2	3.13	117.38	110.34
5	C	2004	OBN	C1'-O3-C3	3.16	122.14	115.01
9	A	1109	17F	O9-C5-C4	3.18	113.11	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1106	1AT	O5-C5-C6	3.19	113.12	106.61
8	A	1107	1DS	O5-C5-C6	3.21	114.46	106.36
6	C	2005	CLR	C11-C9-C10	3.24	117.40	113.11
6	G	1001	CLR	C17-C13-C14	3.33	104.01	100.09
6	E	2001	CLR	C17-C13-C14	3.39	104.08	100.09
9	A	1109	17F	O6-C4-C5	3.40	121.49	109.09
9	A	1108	17F	O9-C5-C4	3.42	113.65	105.90
5	C	2004	OBN	C1'-O5'-C5'	3.46	119.53	113.64
5	A	1104	OBN	C1'-O5'-C5'	3.46	119.55	113.64
6	A	1105	CLR	C7-C8-C14	3.47	116.27	110.86
5	A	1104	OBN	O5'-C5'-C4'	3.52	115.62	109.53
9	B	1005	17F	O9-C5-C4	3.58	114.02	105.90
8	A	1107	1DS	O1-C2'-C3'	3.73	121.04	108.04
6	G	1001	CLR	C7-C8-C14	3.91	116.95	110.86
6	E	2001	CLR	C7-C8-C14	3.93	116.98	110.86
7	A	1106	1AT	O6-C1N-C2N	4.16	124.58	111.90
6	E	2001	CLR	C21-C20-C17	4.17	119.90	112.96
6	G	1001	CLR	C21-C20-C17	4.31	120.13	112.96
6	G	1001	CLR	C1-C10-C9	4.42	114.33	108.64
9	D	2004	17F	O9-C17-C18	4.51	121.33	111.53
8	A	1107	1DS	C2'-O1-C1	4.55	129.52	117.53
6	E	2001	CLR	C1-C10-C9	4.61	114.56	108.64
7	A	1106	1AT	O1-C2'-C3'	4.61	124.10	108.04
5	C	2004	OBN	O5'-C5'-C4'	4.70	117.68	109.53
9	B	1005	17F	O3-C1-C2	4.72	111.62	108.18
6	C	2005	CLR	C7-C8-C14	4.74	118.26	110.86
7	A	1106	1AT	O1-C1-C2	4.75	124.20	108.36
6	A	1105	CLR	C1-C10-C9	4.75	114.75	108.64
6	E	2001	CLR	C7-C8-C9	4.77	116.22	109.71
9	D	2004	17F	C5-O9-C17	4.83	129.47	117.89
6	G	1001	CLR	C7-C8-C9	5.02	116.55	109.71
6	C	2005	CLR	C17-C13-C14	5.04	106.01	100.09
9	G	1002	17F	C6-O7-C7	5.18	131.33	116.85
6	C	2005	CLR	C1-C10-C9	5.21	115.33	108.64
9	B	1005	17F	O9-C17-C18	5.24	122.92	111.53
6	C	2005	CLR	C7-C8-C9	5.35	117.00	109.71
8	A	1107	1DS	C1'-O1'-C1N	5.58	127.84	116.95
9	A	1109	17F	O9-C17-C18	5.66	121.78	111.10
6	A	1105	CLR	C7-C8-C9	5.69	117.47	109.71
8	A	1107	1DS	O2-C2-C3	5.69	123.16	110.34
7	A	1106	1AT	O2-C2-C1	6.07	123.32	110.02
9	G	1002	17F	C5-O9-C17	6.61	130.38	117.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1108	17F	O9-C17-C18	6.62	123.60	111.10
9	A	1108	17F	O3-C1-C2	7.99	114.02	108.18
9	A	1109	17F	O3-C1-C2	8.98	114.73	108.18
9	G	1002	17F	O3-C1-C2	9.03	114.78	108.18
9	B	1005	17F	C5-O9-C17	9.48	130.15	117.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1109	17F	C17-O9-C5-C6

There are no ring outliers.

14 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1104	OBN	10	0
6	A	1105	CLR	5	0
7	A	1106	1AT	6	0
8	A	1107	1DS	6	0
9	A	1108	17F	6	0
9	A	1109	17F	2	0
10	A	1110	CE1	18	0
9	B	1005	17F	2	0
5	C	2004	OBN	6	0
6	C	2005	CLR	2	0
6	E	2001	CLR	4	0
10	E	2002	CE1	1	0
6	G	1001	CLR	4	0
9	G	1002	17F	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{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>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	995/1021 (97%)	0.04	39 (3%) 43 38	51, 91, 218, 288	0
1	C	995/1021 (97%)	0.26	86 (8%) 13 13	58, 126, 273, 342	0
2	B	289/303 (95%)	0.12	16 (5%) 29 26	67, 151, 221, 258	0
2	D	287/303 (94%)	0.35	22 (7%) 16 16	63, 136, 210, 241	0
3	E	32/65 (49%)	-0.47	0 100 100	72, 81, 120, 147	0
3	G	32/65 (49%)	-0.12	1 (3%) 52 48	64, 83, 134, 141	0
All	All	2630/2778 (94%)	0.16	164 (6%) 24 22	51, 116, 242, 342	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	217	ARG	15.0
2	D	218	ASP	10.8
1	C	491	THR	8.5
1	C	545	VAL	8.3
1	A	471	VAL	7.7
1	C	489	PRO	7.6
1	C	470	ILE	7.4
1	C	487	LYS	6.7
1	C	538	LEU	6.6
1	C	471	VAL	6.5
1	C	579	VAL	6.1
1	C	515	LEU	6.1
1	A	470	ILE	6.0
1	C	578	PHE	5.9
1	C	467	TYR	5.9
1	C	539	GLY	5.7
1	C	582	ILE	5.5
1	A	553	LEU	5.4
1	C	553	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	496	HIS	5.4
1	C	385	TRP	5.4
1	C	490	ASN	5.3
2	B	218	ASP	5.3
1	A	483	LEU	5.2
1	C	468	THR	5.2
1	A	500	MET	5.1
1	C	419	GLY	5.0
2	D	219	GLU	5.0
1	C	576	LEU	4.9
1	C	552	PHE	4.8
1	A	474	PRO	4.7
1	A	564	PHE	4.6
1	C	535	TYR	4.6
1	C	420	LEU	4.6
1	A	496	HIS	4.6
1	A	473	ILE	4.4
1	C	497	LEU	4.4
1	C	571	PHE	4.4
1	C	492	ALA	4.3
1	C	550	HIS	4.2
1	C	580	GLY	4.2
1	C	518	GLY	4.2
1	C	466	ARG	4.2
1	C	514	ILE	4.1
1	C	548	PHE	4.1
1	C	581	LEU	4.1
1	C	519	LYS	4.0
2	D	23	GLU	4.0
1	C	551	LEU	4.0
1	A	486	HIS	4.0
2	D	274	ILE	4.0
2	D	178	ILE	3.9
1	A	580	GLY	3.9
1	A	480	LYS	3.8
1	C	426	PHE	3.8
2	B	217	ARG	3.8
1	A	548	PHE	3.7
1	C	22	GLU	3.7
1	A	472	GLU	3.7
1	C	575	ASN	3.7
2	B	199	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	571	PHE	3.6
2	D	176	VAL	3.6
1	A	581	LEU	3.6
1	C	384	MET	3.6
2	D	77	LEU	3.6
1	C	549	CYS	3.6
1	C	522	PRO	3.5
1	C	119	GLN	3.5
1	A	485	ILE	3.4
1	A	482	GLN	3.4
1	C	520	GLU	3.4
1	C	437	LYS	3.4
2	D	220	ASP	3.4
1	C	536	LEU	3.3
1	C	546	LEU	3.3
1	A	499	VAL	3.3
1	C	488	ASN	3.3
1	C	440	VAL	3.3
1	A	484	SER	3.3
1	A	475	PHE	3.3
1	A	498	LEU	3.3
1	C	486	HIS	3.2
2	B	196	LEU	3.2
1	C	441	ALA	3.2
1	C	527	LEU	3.2
1	A	477	SER	3.2
2	B	163	ASN	3.1
1	A	545	VAL	3.1
1	C	498	LEU	3.1
2	B	198	THR	3.1
1	A	497	LEU	3.0
2	B	243	TYR	3.0
1	C	494	PRO	2.9
1	C	573	LEU	2.9
1	C	547	GLY	2.9
2	D	199	TYR	2.9
1	A	385	TRP	2.9
1	A	534	ALA	2.8
1	C	566	THR	2.8
1	A	501	LYS	2.8
1	C	531	PHE	2.7
1	A	120	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	195	SER	2.7
1	C	528	LYS	2.7
1	C	25	MET	2.7
1	C	430	GLN	2.7
2	B	162	LEU	2.6
1	A	21	LYS	2.6
1	C	534	ALA	2.6
1	A	578	PHE	2.6
1	C	68	ASP	2.6
1	C	469	LYS	2.6
1	C	485	ILE	2.6
2	D	277	LYS	2.5
1	C	418	ALA	2.5
2	B	139	TYR	2.5
2	D	255	LEU	2.5
1	C	432	ASN	2.5
2	D	263	PHE	2.5
2	D	275	GLU	2.5
1	C	507	ILE	2.5
1	C	428	ALA	2.5
1	A	579	VAL	2.5
1	C	30	LYS	2.5
1	A	429	ASN	2.4
1	A	428	ALA	2.4
2	D	260	ALA	2.4
1	C	202	ASN	2.4
1	C	529	ASP	2.3
1	C	532	GLN	2.3
1	C	26	ASP	2.3
2	B	278	ALA	2.3
1	C	577	CYS	2.3
2	B	212	HIS	2.3
1	C	701	GLN	2.3
1	C	509	ASP	2.3
2	D	297	VAL	2.3
1	A	487	LYS	2.3
2	B	183	VAL	2.2
1	C	465	GLU	2.2
2	D	98	TYR	2.2
2	D	162	LEU	2.2
2	D	177	ILE	2.2
2	D	259	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	572	PRO	2.2
1	C	146	LYS	2.2
1	C	393	ALA	2.2
2	D	237	GLY	2.2
1	C	404	PHE	2.2
1	A	479	ASN	2.2
1	A	538	LEU	2.1
3	G	19	PHE	2.1
1	C	511	CYS	2.1
1	C	642	ASN	2.1
1	A	566	THR	2.1
2	B	15	PHE	2.1
2	D	211	VAL	2.1
1	C	120	ASN	2.1
1	C	29	LYS	2.1
1	A	386	SER	2.1
2	B	186	PHE	2.1
1	C	708	THR	2.0
2	B	174	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{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	LLDF	B-factors(Å^2)	Q<0.9
1	PHD	C	369	12/13	0.98	0.18	-	107,112,123,124	0
1	PHD	A	369	12/13	0.98	0.17	-	66,71,74,75	0

6.3 Carbohydrates (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^{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	LLDF	B-factors(Å^2)	Q<0.9
11	NAG	B	1001	14/15	0.82	0.18	-	179,192,203,207	0
11	NAG	B	1002	14/15	0.72	0.41	-	205,218,224,229	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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^{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	LLDF	B-factors(Å^2)	Q<0.9
4	MG	A	1102	1/1	0.97	0.41	14.72	82,82,82,82	0
6	CLR	C	2005	28/28	0.84	0.49	5.32	93,104,113,231	0
9	17F	D	2004	28/54	0.82	0.47	4.78	154,172,243,246	0
9	17F	G	1002	27/54	0.71	0.39	4.15	83,124,256,258	0
10	CE1	E	2002	22/37	0.86	0.36	3.82	67,109,155,157	0
9	17F	A	1109	18/54	0.84	0.32	3.25	96,114,166,169	0
10	CE1	A	1110	34/37	0.87	0.30	2.84	79,110,144,146	0
9	17F	A	1108	18/54	0.84	0.32	2.74	80,155,188,197	0
9	17F	B	1005	24/54	0.78	0.28	2.64	74,128,199,208	0
4	MG	C	2002	1/1	0.97	0.34	2.60	124,124,124,124	0
6	CLR	E	2001	28/28	0.96	0.25	0.81	64,71,73,73	0
6	CLR	A	1105	28/28	0.93	0.26	0.27	74,112,143,159	0
6	CLR	G	1001	28/28	0.97	0.20	0.00	57,66,79,83	0
5	OBN	A	1104	41/41	0.95	0.19	-0.33	72,81,85,88	0
5	OBN	C	2004	41/41	0.94	0.19	-0.41	84,92,99,104	0
4	MG	A	1101	1/1	0.96	0.19	-0.61	113,113,113,113	0
4	MG	C	2001	1/1	0.98	0.20	-0.70	147,147,147,147	0
7	1AT	A	1106	29/34	0.94	0.19	-0.81	85,99,116,118	0
8	1DS	A	1107	29/34	0.93	0.20	-0.99	56,123,141,170	0
4	MG	A	1103	1/1	0.95	0.22	-1.10	58,58,58,58	0
4	MG	C	2003	1/1	0.92	0.20	-1.61	81,81,81,81	0
12	NAG	D	2001	14/15	0.85	0.22	-	138,159,173,175	0
12	NAG	D	2003	14/15	0.80	0.32	-	191,198,211,218	0
12	NAG	B	1003	14/15	0.71	0.22	-	197,209,221,225	0
12	NAG	D	2002	14/15	0.79	0.14	-	142,150,163,169	0
12	NAG	B	1004	14/15	0.74	0.45	-	199,203,212,213	0

6.5 Other polymers (i)

There are no such residues in this entry.