Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:19 am BST

PDB ID	:	1W1W
Title	:	Sc Smc1hd:Scc1-C complex, ATPgS
Authors	:	Haering, C.; Nasmyth, K.; Lowe, J.
Deposited on	:	2004-06-24
Resolution	:	2.90 Å(reported)

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

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

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

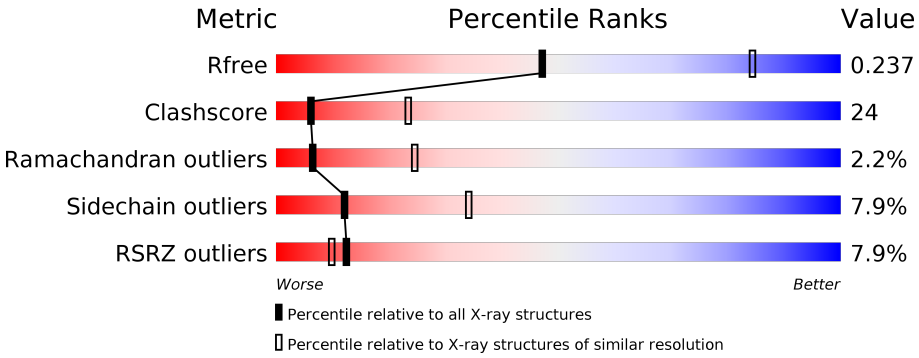
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	430	9% 36% 24% · 36%
1	B	430	5% 45% 26% · 24%
1	C	430	3% 45% 27% · 24%
1	D	430	7% 44% 26% 6% 24%
2	E	121	9% 30% 25% · 41%
2	F	121	6% 32% 23% · 41%

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Mol	Chain	Length	Quality of chain
2	G	121	2% 28% 26% 41%
2	H	121	2% 36% 19% 41%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12360 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 STRUCTURAL MAINTENANCE OF CHROMOSOME 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2175	1394	365	410	6			
1	B	327	Total	C	N	O	S	0	0	0
			2627	1684	439	498	6			
1	C	327	Total	C	N	O	S	0	0	0
			2627	1684	439	498	6			
1	D	327	Total	C	N	O	S	0	0	0
			2627	1684	439	498	6			

- Molecule 2 is a protein called SISTER CHROMATID COHESION PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	71	Total	C	N	O	S	0	0	1
			544	348	92	102	2			
2	F	71	Total	C	N	O	S	0	0	1
			544	348	92	102	2			
2	G	71	Total	C	N	O	S	0	0	1
			544	348	92	102	2			
2	H	71	Total	C	N	O	S	0	0	1
			544	348	92	102	2			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	444	MET	-	expression tag	UNP Q12158
E	445	HIS	-	expression tag	UNP Q12158
E	446	HIS	-	expression tag	UNP Q12158
E	447	HIS	-	expression tag	UNP Q12158
E	448	HIS	-	expression tag	UNP Q12158
E	449	HIS	-	expression tag	UNP Q12158
E	450	HIS	-	expression tag	UNP Q12158
F	444	MET	-	expression tag	UNP Q12158

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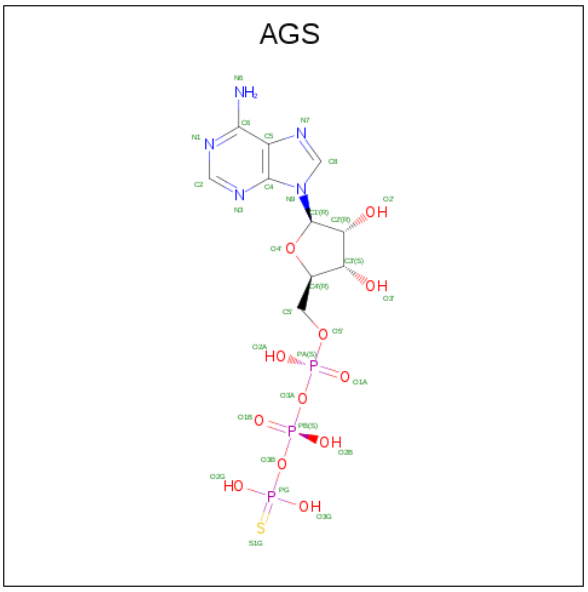
Chain	Residue	Modelled	Actual	Comment	Reference
F	445	HIS	-	expression tag	UNP Q12158
F	446	HIS	-	expression tag	UNP Q12158
F	447	HIS	-	expression tag	UNP Q12158
F	448	HIS	-	expression tag	UNP Q12158
F	449	HIS	-	expression tag	UNP Q12158
F	450	HIS	-	expression tag	UNP Q12158
G	444	MET	-	expression tag	UNP Q12158
G	445	HIS	-	expression tag	UNP Q12158
G	446	HIS	-	expression tag	UNP Q12158
G	447	HIS	-	expression tag	UNP Q12158
G	448	HIS	-	expression tag	UNP Q12158
G	449	HIS	-	expression tag	UNP Q12158
G	450	HIS	-	expression tag	UNP Q12158
H	444	MET	-	expression tag	UNP Q12158
H	445	HIS	-	expression tag	UNP Q12158
H	446	HIS	-	expression tag	UNP Q12158
H	447	HIS	-	expression tag	UNP Q12158
H	448	HIS	-	expression tag	UNP Q12158
H	449	HIS	-	expression tag	UNP Q12158
H	450	HIS	-	expression tag	UNP Q12158

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



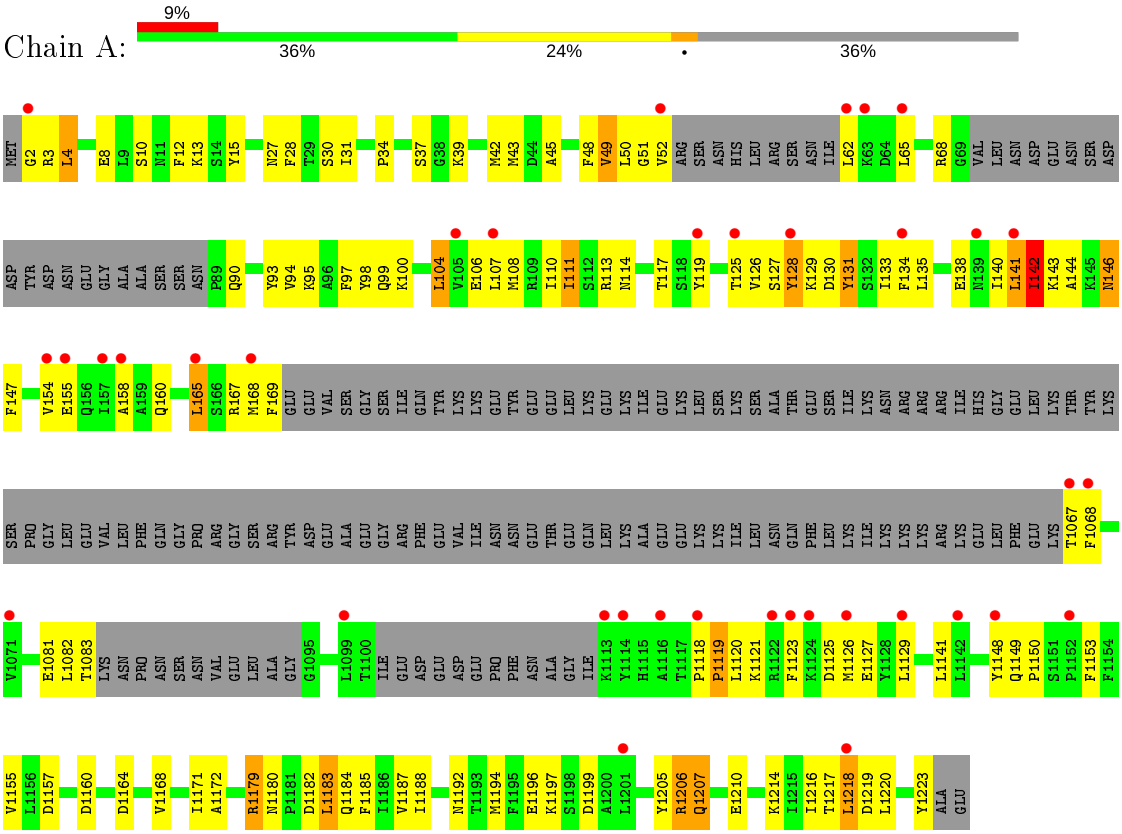
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

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

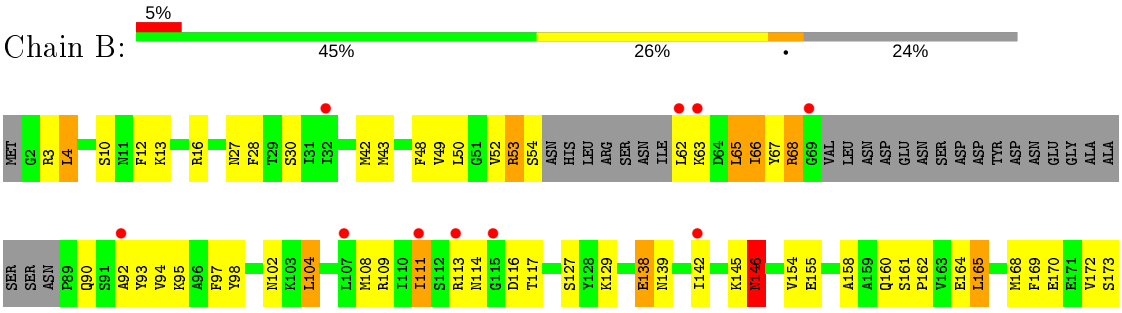
- Molecule 1: STRUCTURAL MAINTENANCE OF CHROMOSOME 1

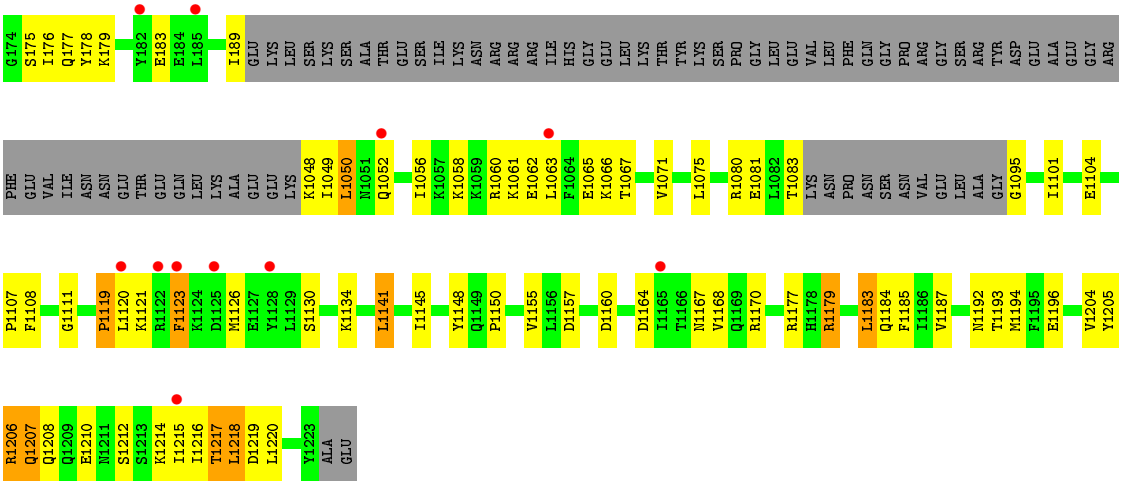
Chain A:



- Molecule 1: STRUCTURAL MAINTENANCE OF CHROMOSOME 1

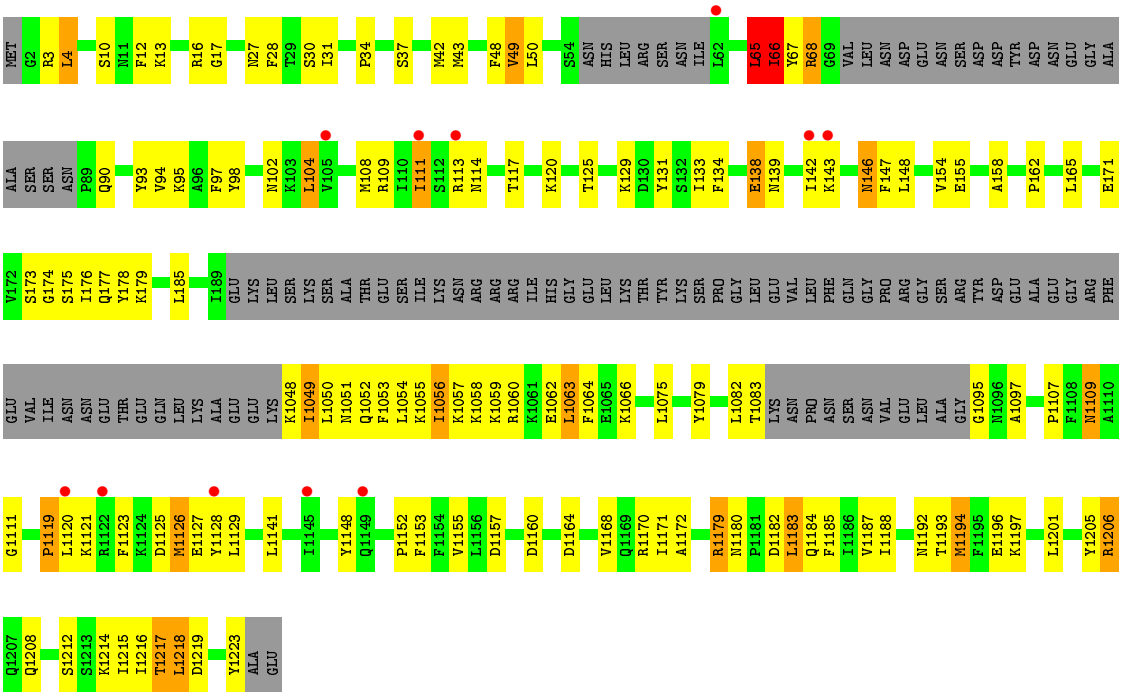
Chain B:





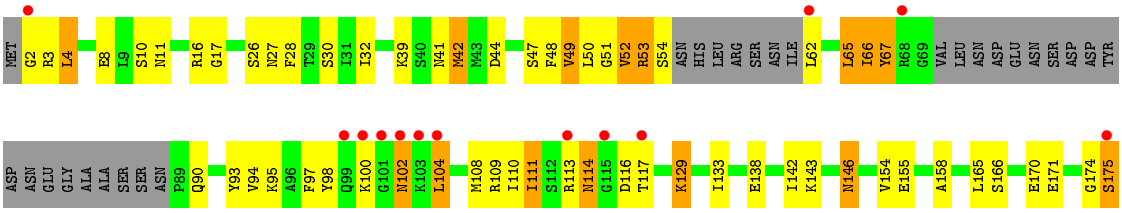
• Molecule 1: STRUCTURAL MAINTENANCE OF CHROMOSOME 1

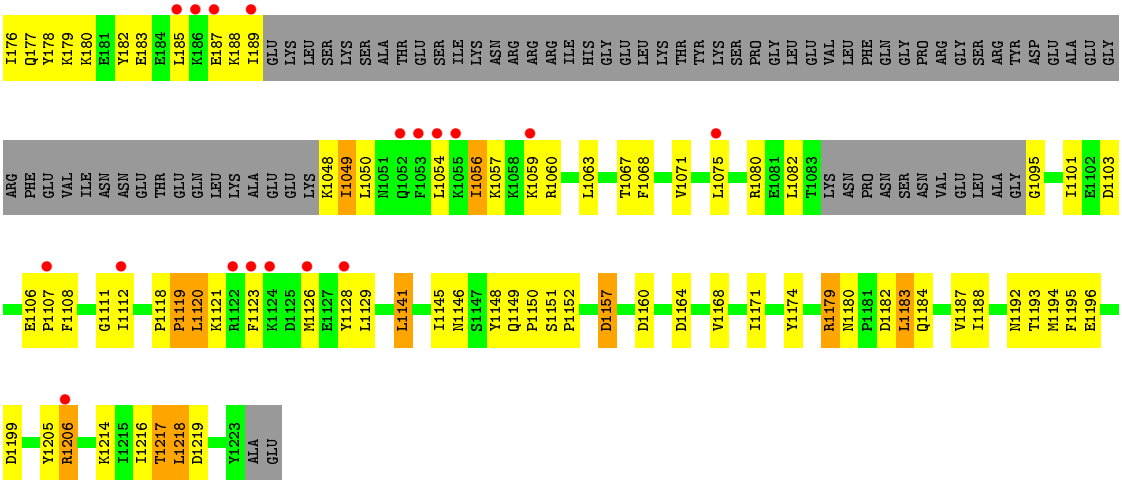
Chain C:



• Molecule 1: STRUCTURAL MAINTENANCE OF CHROMOSOME 1

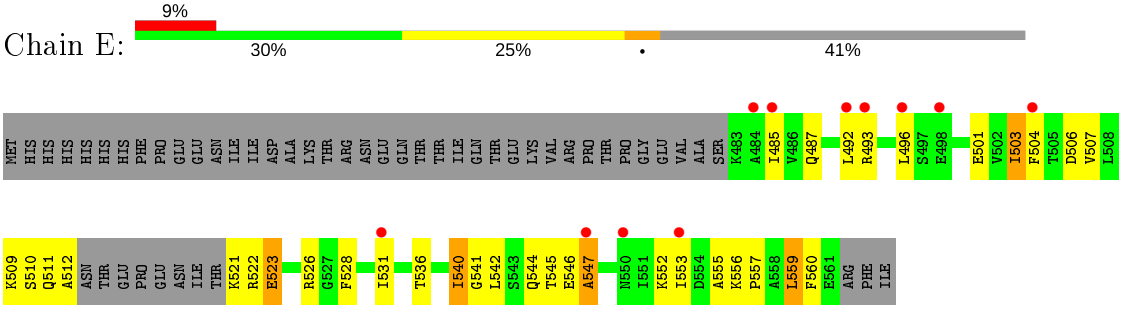
Chain D:





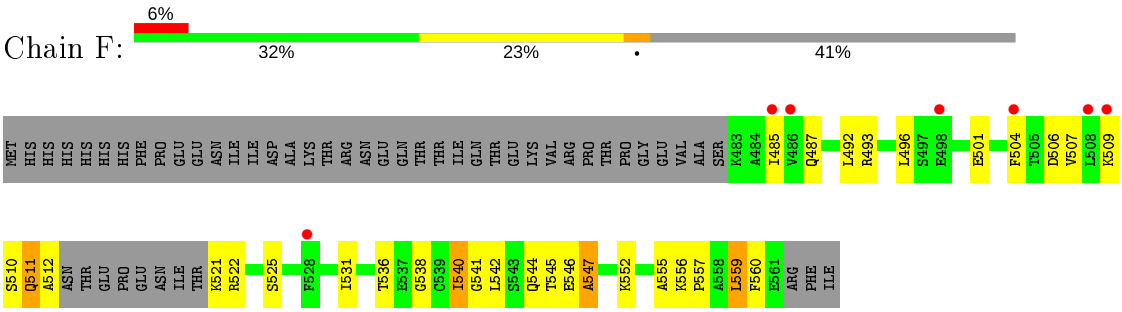
- Molecule 2: SISTER CHROMATID COHESION PROTEIN 1

Chain E:



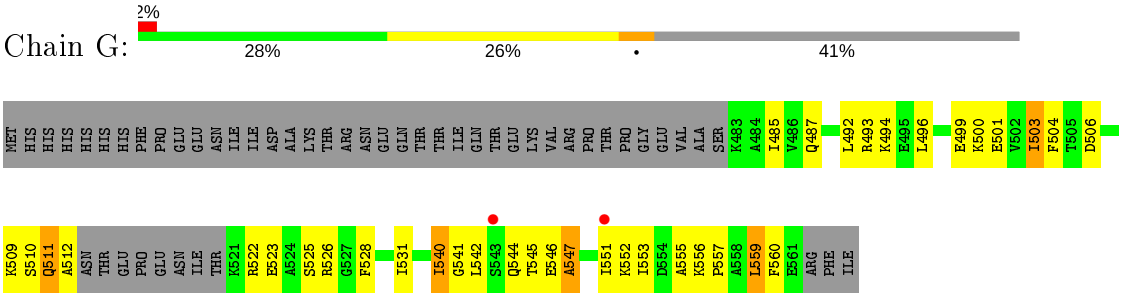
- Molecule 2: SISTER CHROMATID COHESION PROTEIN 1

Chain F:



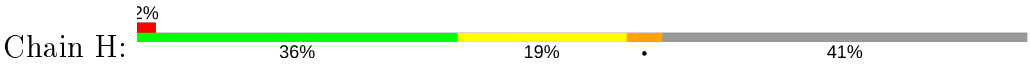
- Molecule 2: SISTER CHROMATID COHESION PROTEIN 1

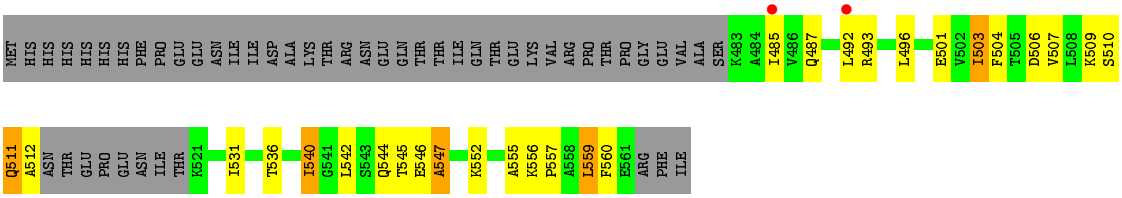
Chain G:



- Molecule 2: SISTER CHROMATID COHESION PROTEIN 1

Chain H:




MET HIS HIS HIS HIS HIS PHE PRO GLU GLU ASN ILE ILE ASP ALA LYS THR ARG ASN GLU GLN THR THR ILE GLN THR GLU LYS VAL ARG PRO THR PRO GLY GLU VAL ALA SER K483 A484 I485 V486 Q487 L492 R493 L496 E501 V502 I503 F504 T505 D506 V507 L508 K509 S510
Q511 A512 ASN THR GLU PRO GLU ASN ILE THR K521 I531 T536 I540 G541 L542 S543 Q544 T545 E546 A547 K552 A555 K556 P557 A558 L559 F560 E561 ARG PHE ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	138.47Å 138.47Å 284.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 284.07 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.90) 98.8 (284.07-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.275 0.235 , 0.237	Depositor DCC
R_{free} test set	3145 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	70.4	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12360	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, AGS

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	0.46	0/2211	0.71	0/2974
1	B	0.43	0/2670	0.69	1/3583 (0.0%)
1	C	0.45	0/2670	0.71	1/3583 (0.0%)
1	D	0.46	0/2670	0.70	1/3583 (0.0%)
2	E	0.41	0/548	0.55	0/730
2	F	0.42	0/548	0.57	0/730
2	G	0.45	0/548	0.58	0/730
2	H	0.48	0/548	0.60	0/730
All	All	0.45	0/12413	0.68	3/16643 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	65	LEU	N-CA-C	-6.12	94.47	111.00
1	B	65	LEU	N-CA-C	-5.17	97.05	111.00
1	D	65	LEU	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2175	0	2182	131	0
1	B	2627	0	2651	131	0
1	C	2627	0	2651	118	0
1	D	2627	0	2651	135	0
2	E	544	0	570	34	0
2	F	544	0	570	29	0
2	G	544	0	570	41	0
2	H	544	0	570	30	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
4	A	31	0	12	3	0
4	B	31	0	12	0	0
4	C	31	0	12	1	0
4	D	31	0	12	1	0
All	All	12360	0	12463	608	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 24.

All (608) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:496:LEU:HD13	2:G:555:ALA:HB2	1.33	1.07
2:H:496:LEU:HD13	2:H:555:ALA:HB2	1.34	1.06
2:E:496:LEU:HD13	2:E:555:ALA:HB2	1.43	1.00
1:B:54:SER:HA	1:B:145:LYS:HZ1	1.28	0.99
1:C:1206:ARG:HH21	1:C:1206:ARG:HB3	1.26	0.99
1:B:1206:ARG:HH21	1:B:1206:ARG:HB3	1.29	0.98
2:F:496:LEU:HD13	2:F:555:ALA:HB2	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:H	1:A:1184:GLN:HE22	1.08	0.95
2:E:504:PHE:CD1	2:E:531:ILE:HD11	2.05	0.91
1:D:1206:ARG:HH21	1:D:1206:ARG:HB3	1.33	0.91
1:D:4:LEU:H	1:D:1184:GLN:HE22	1.12	0.90
1:C:4:LEU:H	1:C:1184:GLN:HE22	1.18	0.89
1:B:179:LYS:HD3	1:B:1060:ARG:NH1	1.88	0.89
1:D:1217:THR:H	2:H:544:GLN:HE22	1.14	0.89
1:A:1206:ARG:HH21	1:A:1206:ARG:HB3	1.37	0.88
1:B:4:LEU:H	1:B:1184:GLN:HE22	1.20	0.87
1:A:126:VAL:HB	1:A:130:ASP:HB2	1.57	0.86
1:C:1217:THR:H	2:G:544:GLN:HE22	1.18	0.86
2:H:504:PHE:CD1	2:H:531:ILE:HD11	2.11	0.84
2:G:504:PHE:CD1	2:G:531:ILE:HD11	2.12	0.84
1:C:1206:ARG:HH21	1:C:1206:ARG:CB	1.91	0.83
1:A:1217:THR:H	2:E:544:GLN:HE22	1.21	0.83
1:A:1206:ARG:HB2	2:E:536:THR:HG23	1.60	0.83
1:B:54:SER:HA	1:B:145:LYS:NZ	1.94	0.82
1:A:12:PHE:O	1:A:65:LEU:O	1.97	0.81
1:A:146:ASN:H	1:A:146:ASN:HD22	1.25	0.81
1:C:43:MET:HG3	1:C:1155:VAL:HG11	1.63	0.80
1:A:50:LEU:O	1:A:142:ILE:HG12	1.82	0.79
1:A:1083:THR:HG21	1:A:1119:PRO:HD3	1.65	0.79
2:F:504:PHE:CD1	2:F:531:ILE:HD11	2.17	0.79
1:D:174:GLY:O	1:D:177:GLN:HG2	1.83	0.78
1:B:1217:THR:H	2:F:544:GLN:HE22	1.30	0.78
2:E:545:THR:HG22	2:E:546:GLU:HG3	1.65	0.78
1:D:1206:ARG:CB	1:D:1206:ARG:HH21	1.96	0.77
1:D:3:ARG:HE	1:D:27:ASN:HD21	1.33	0.76
1:C:3:ARG:HE	1:C:27:ASN:HD21	1.32	0.76
1:B:162:PRO:HB2	1:B:1111:GLY:HA3	1.66	0.76
1:D:189:ILE:H	1:D:189:ILE:HD12	1.49	0.76
1:D:1057:LYS:HD2	1:D:1106:GLU:OE1	1.86	0.76
1:D:178:TYR:HB2	1:D:1060:ARG:HD2	1.68	0.75
2:H:492:LEU:HD13	2:H:540:ILE:CD1	2.17	0.75
2:G:492:LEU:HD13	2:G:540:ILE:CD1	2.17	0.75
1:D:3:ARG:HE	1:D:27:ASN:ND2	1.84	0.75
1:A:142:ILE:H	1:A:142:ILE:HD12	1.52	0.74
1:A:3:ARG:HE	1:A:27:ASN:HD21	1.35	0.74
2:G:531:ILE:HG22	2:G:542:LEU:HD11	1.70	0.74
1:C:50:LEU:O	1:C:142:ILE:HG21	1.87	0.74
1:D:1119:PRO:O	1:D:1121:LYS:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:531:ILE:HG22	2:H:542:LEU:HD11	1.70	0.73
1:C:143:LYS:HG2	1:C:171:GLU:HG3	1.70	0.73
1:B:50:LEU:O	1:B:142:ILE:HG21	1.88	0.73
1:A:1206:ARG:HH21	1:A:1206:ARG:CB	2.01	0.73
1:B:1061:LYS:O	1:B:1065:GLU:HG3	1.88	0.72
1:C:1206:ARG:NH2	1:C:1206:ARG:HB3	2.04	0.72
1:D:50:LEU:O	1:D:142:ILE:HG21	1.89	0.72
1:D:95:LYS:HE2	1:D:108:MET:CE	2.20	0.72
1:A:1192:ASN:HD21	2:E:526:ARG:HD2	1.54	0.72
2:E:531:ILE:HG22	2:E:542:LEU:HD11	1.72	0.72
1:A:126:VAL:HB	1:A:130:ASP:CB	2.20	0.72
1:B:170:GLU:HG3	1:B:175:SER:OG	1.89	0.72
1:D:109:ARG:HH11	1:D:117:THR:HG21	1.53	0.71
1:C:1217:THR:N	2:G:544:GLN:HE22	1.88	0.71
1:C:3:ARG:HE	1:C:27:ASN:ND2	1.88	0.71
1:C:146:ASN:HD22	1:C:146:ASN:H	1.38	0.70
1:D:189:ILE:HD12	1:D:189:ILE:N	2.06	0.70
1:B:1206:ARG:HH21	1:B:1206:ARG:CB	2.03	0.70
2:F:492:LEU:HD13	2:F:540:ILE:CD1	2.21	0.70
1:B:43:MET:HG3	1:B:1155:VAL:HG11	1.74	0.69
1:C:1179:ARG:C	1:C:1179:ARG:HD2	2.13	0.69
1:C:48:PHE:HZ	1:C:111:ILE:HG12	1.58	0.69
1:B:53:ARG:HD3	1:B:53:ARG:O	1.92	0.68
2:F:531:ILE:HG22	2:F:542:LEU:HD11	1.74	0.68
1:D:1217:THR:N	2:H:544:GLN:HE22	1.90	0.68
1:A:140:ILE:O	1:A:142:ILE:HG13	1.93	0.68
2:E:492:LEU:HD13	2:E:540:ILE:CD1	2.23	0.68
1:A:142:ILE:N	1:A:142:ILE:HD12	2.09	0.68
1:D:95:LYS:HE2	1:D:108:MET:HE2	1.75	0.67
2:H:492:LEU:HD13	2:H:540:ILE:HD11	1.75	0.67
1:A:1067:THR:HG23	1:A:1148:TYR:CD2	2.30	0.67
1:A:142:ILE:H	1:A:142:ILE:CD1	2.04	0.67
1:B:90:GLN:OE1	1:B:113:ARG:HD2	1.95	0.67
1:B:109:ARG:HH11	1:B:117:THR:HG21	1.58	0.67
1:C:1048:LYS:C	1:C:1048:LYS:HD3	2.16	0.67
1:A:146:ASN:N	1:A:146:ASN:HD22	1.92	0.66
1:A:3:ARG:HE	1:A:27:ASN:ND2	1.92	0.66
1:D:189:ILE:H	1:D:189:ILE:CD1	2.09	0.66
1:B:1160:ASP:OD2	1:B:1194:MET:HG3	1.96	0.66
1:B:1183:LEU:HD13	1:B:1185:PHE:CE1	2.31	0.66
1:B:48:PHE:HZ	1:B:111:ILE:HG12	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:TYR:HB3	1:A:131:TYR:CD1	2.31	0.66
1:B:3:ARG:HE	1:B:27:ASN:HD21	1.43	0.66
2:F:501:GLU:OE1	2:F:552:LYS:HD3	1.95	0.66
2:E:506:ASP:O	2:E:509:LYS:HB3	1.96	0.66
1:B:1164:ASP:O	1:B:1168:VAL:HG23	1.96	0.65
1:C:1050:LEU:O	1:C:1050:LEU:HD23	1.95	0.65
1:C:90:GLN:OE1	1:C:113:ARG:HD2	1.96	0.65
2:G:496:LEU:HD13	2:G:555:ALA:CB	2.20	0.65
1:D:179:LYS:HA	1:D:1060:ARG:HH22	1.61	0.65
1:D:1068:PHE:CE1	1:D:1112:ILE:HD12	2.31	0.65
1:D:1164:ASP:O	1:D:1168:VAL:HG23	1.97	0.65
1:A:169:PHE:CZ	1:A:1068:PHE:HD1	2.14	0.65
1:B:95:LYS:HE2	1:B:108:MET:CE	2.27	0.65
1:A:52:VAL:CG2	1:A:142:ILE:HB	2.28	0.64
1:C:109:ARG:HH11	1:C:117:THR:HG21	1.62	0.64
1:A:1192:ASN:ND2	2:E:526:ARG:HD2	2.12	0.64
1:B:48:PHE:CZ	1:B:111:ILE:HG12	2.33	0.64
1:C:177:GLN:HG3	1:C:178:TYR:N	2.13	0.64
1:C:48:PHE:CZ	1:C:111:ILE:HG12	2.32	0.64
1:B:3:ARG:HE	1:B:27:ASN:ND2	1.95	0.64
2:F:506:ASP:O	2:F:509:LYS:HB3	1.98	0.64
1:A:1217:THR:N	2:E:544:GLN:HE22	1.96	0.63
1:B:98:TYR:CE2	1:B:138:GLU:HG2	2.34	0.63
1:A:48:PHE:CZ	1:A:111:ILE:HG12	2.33	0.63
1:D:146:ASN:HD22	1:D:146:ASN:H	1.45	0.63
1:D:1206:ARG:CG	1:D:1206:ARG:HH21	2.11	0.63
2:G:504:PHE:HD1	2:G:531:ILE:HD11	1.61	0.63
1:B:1119:PRO:O	1:B:1121:LYS:N	2.31	0.63
1:B:63:LYS:HE2	1:B:113:ARG:HG2	1.81	0.63
1:D:179:LYS:HA	1:D:1060:ARG:NH2	2.15	0.62
1:C:1217:THR:OG1	2:G:547:ALA:O	2.17	0.62
1:C:1083:THR:CG2	1:C:1119:PRO:HD3	2.29	0.62
2:E:503:ILE:HG22	2:E:506:ASP:H	1.64	0.62
1:C:1083:THR:HG23	1:C:1119:PRO:HD3	1.81	0.62
1:C:1183:LEU:HD13	1:C:1185:PHE:CE1	2.34	0.62
1:D:1206:ARG:NH2	1:D:1206:ARG:HB3	2.10	0.62
1:D:188:LYS:HZ3	1:D:1049:ILE:HG12	1.64	0.62
2:G:496:LEU:CD1	2:G:555:ALA:HB2	2.22	0.62
1:B:189:ILE:N	1:B:189:ILE:HD12	2.14	0.62
2:F:510:SER:O	2:F:511:GLN:HG3	2.00	0.62
1:A:129:LYS:O	1:A:129:LYS:HD3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1164:ASP:O	1:C:1168:VAL:HG23	2.00	0.61
1:A:107:LEU:HD21	1:A:134:PHE:CE2	2.35	0.61
1:B:1066:LYS:HG2	1:B:1148:TYR:OH	2.00	0.61
2:F:531:ILE:CG2	2:F:542:LEU:HD21	2.30	0.61
1:C:1206:ARG:HH21	1:C:1206:ARG:CG	2.13	0.61
1:D:170:GLU:HB3	1:D:176:ILE:HB	1.82	0.61
1:D:51:GLY:O	1:D:52:VAL:HB	2.01	0.61
1:D:90:GLN:OE1	1:D:113:ARG:HD2	2.00	0.61
1:B:1206:ARG:HB2	2:F:536:THR:HG23	1.82	0.61
1:D:143:LYS:HG2	1:D:171:GLU:HG3	1.82	0.60
1:A:48:PHE:HZ	1:A:111:ILE:HG12	1.66	0.60
2:G:501:GLU:OE1	2:G:552:LYS:HD3	2.01	0.60
4:C:2224:AGS:H3'	1:D:1128:TYR:O	2.01	0.60
1:B:176:ILE:O	1:B:179:LYS:HB3	2.02	0.60
2:H:503:ILE:HG22	2:H:506:ASP:H	1.65	0.60
1:A:1179:ARG:HD2	1:A:1179:ARG:C	2.21	0.60
1:A:1206:ARG:HH21	1:A:1206:ARG:CG	2.15	0.60
2:H:504:PHE:HD1	2:H:531:ILE:HD11	1.66	0.60
1:A:1164:ASP:O	1:A:1168:VAL:HG23	2.02	0.59
1:B:173:SER:HB3	1:B:1067:THR:HB	1.83	0.59
1:B:146:ASN:HD22	1:B:146:ASN:H	1.50	0.59
1:C:1119:PRO:O	1:C:1121:LYS:N	2.34	0.59
1:D:188:LYS:NZ	1:D:1049:ILE:HG12	2.17	0.59
1:B:66:ILE:HD13	1:B:92:ALA:CB	2.32	0.59
2:E:501:GLU:OE1	2:E:552:LYS:HD3	2.03	0.59
2:F:504:PHE:HD1	2:F:531:ILE:HD11	1.63	0.59
1:A:140:ILE:O	1:A:140:ILE:HG22	2.02	0.59
2:F:545:THR:HG22	2:F:546:GLU:HG3	1.84	0.59
2:H:510:SER:O	2:H:511:GLN:HG3	2.04	0.58
1:D:53:ARG:C	1:D:53:ARG:HD3	2.24	0.58
1:B:158:ALA:HB1	1:B:1126:MET:CE	2.34	0.58
1:C:1048:LYS:O	1:C:1048:LYS:HD3	2.03	0.58
1:C:1128:TYR:O	4:D:2224:AGS:H3'	2.04	0.58
1:A:1183:LEU:HD13	1:A:1185:PHE:CE1	2.38	0.58
2:H:496:LEU:HD13	2:H:555:ALA:CB	2.21	0.58
1:B:66:ILE:HD13	1:B:92:ALA:N	2.19	0.58
1:D:39:LYS:O	1:D:42:MET:HB2	2.04	0.58
2:G:545:THR:HG22	2:G:546:GLU:HG3	1.85	0.58
1:A:154:VAL:HG13	1:A:155:GLU:N	2.18	0.57
2:E:531:ILE:CG2	2:E:542:LEU:HD21	2.34	0.57
1:B:95:LYS:HE2	1:B:108:MET:HE2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1101:ILE:HG21	1:D:1107:PRO:HB3	1.85	0.57
1:B:1217:THR:N	2:F:544:GLN:HE22	2.01	0.57
1:D:97:PHE:HB3	1:D:104:LEU:HD21	1.86	0.57
1:D:48:PHE:HZ	1:D:111:ILE:HG12	1.68	0.57
1:C:65:LEU:O	1:C:66:ILE:O	2.23	0.57
1:D:182:TYR:HE1	1:D:1057:LYS:HG3	1.70	0.57
1:C:1208:GLN:NE2	1:D:1120:LEU:HD13	2.20	0.56
1:D:154:VAL:HG13	1:D:155:GLU:N	2.21	0.56
1:C:1216:ILE:HA	2:G:544:GLN:NE2	2.20	0.56
1:C:43:MET:HG3	1:C:1155:VAL:CG1	2.33	0.56
1:D:1148:TYR:CD2	1:D:1149:GLN:HG3	2.40	0.56
1:A:1206:ARG:NH2	1:A:1206:ARG:HB3	2.15	0.56
1:A:1119:PRO:O	1:A:1121:LYS:N	2.38	0.56
4:A:2224:AGS:H5'1	1:B:1130:SER:HB3	1.86	0.56
1:B:12:PHE:CD1	1:B:13:LYS:HG3	2.41	0.56
1:D:1205:TYR:HE2	1:D:1216:ILE:HG23	1.71	0.56
1:C:1205:TYR:HE2	1:C:1216:ILE:HG23	1.71	0.56
1:D:3:ARG:NE	1:D:27:ASN:HD21	2.00	0.56
1:C:178:TYR:CE2	1:C:1059:LYS:HD3	2.40	0.56
1:D:48:PHE:CZ	1:D:111:ILE:HG12	2.41	0.56
1:B:1058:LYS:O	1:B:1062:GLU:HG3	2.06	0.55
1:A:141:LEU:CD2	1:A:144:ALA:H	2.19	0.55
1:B:98:TYR:OH	1:B:138:GLU:HG2	2.07	0.55
1:A:1205:TYR:CZ	1:A:1214:LYS:HB2	2.40	0.55
1:C:185:LEU:HD13	1:C:1052:GLN:HB2	1.88	0.55
1:C:1058:LYS:O	1:C:1062:GLU:HG3	2.07	0.55
2:H:531:ILE:CG2	2:H:542:LEU:HD21	2.37	0.55
1:C:98:TYR:OH	1:C:138:GLU:HG3	2.07	0.55
1:D:1049:ILE:O	1:D:1049:ILE:HG23	2.07	0.55
1:D:1141:LEU:HD22	1:D:1145:ILE:HD11	1.89	0.55
1:A:100:LYS:HE3	1:A:138:GLU:OE2	2.07	0.55
1:C:49:VAL:HG13	1:C:94:VAL:CG1	2.36	0.55
2:H:545:THR:HG22	2:H:546:GLU:HG3	1.87	0.55
1:B:160:GLN:HE22	1:B:168:MET:CE	2.20	0.55
2:G:510:SER:O	2:G:511:GLN:HG3	2.06	0.55
1:A:146:ASN:ND2	1:A:146:ASN:H	2.01	0.55
1:A:62:LEU:O	1:A:65:LEU:HG	2.06	0.55
1:B:102:ASN:N	1:B:102:ASN:HD22	2.05	0.55
1:D:102:ASN:HD22	1:D:102:ASN:N	2.04	0.55
1:D:1048:LYS:C	1:D:1050:LEU:H	2.08	0.55
1:D:1216:ILE:HA	2:H:544:GLN:NE2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:LEU:HD22	1:B:1145:ILE:CD1	2.37	0.55
1:D:110:ILE:O	1:D:117:THR:HA	2.06	0.54
1:A:130:ASP:O	1:A:133:ILE:HG12	2.07	0.54
1:B:1050:LEU:HD23	1:B:1050:LEU:C	2.28	0.54
1:C:158:ALA:HB1	1:C:1126:MET:CE	2.38	0.54
1:A:43:MET:HG3	1:A:1155:VAL:HG11	1.90	0.54
1:D:1118:PRO:HD3	1:D:1129:LEU:HD21	1.88	0.54
1:A:4:LEU:H	1:A:1184:GLN:NE2	1.92	0.54
1:D:1206:ARG:HB2	2:H:536:THR:HG23	1.88	0.54
1:B:189:ILE:HD11	1:B:1049:ILE:HG23	1.90	0.54
1:A:131:TYR:CE2	1:A:135:LEU:HD11	2.43	0.54
1:A:90:GLN:OE1	1:A:113:ARG:HD2	2.07	0.54
1:C:177:GLN:HG3	1:C:178:TYR:H	1.73	0.54
1:D:158:ALA:HB1	1:D:1126:MET:CE	2.38	0.54
2:H:506:ASP:O	2:H:509:LYS:HB3	2.07	0.54
1:A:49:VAL:HG13	1:A:94:VAL:CG1	2.38	0.53
2:G:503:ILE:HG22	2:G:506:ASP:H	1.72	0.53
1:A:1148:TYR:O	1:A:1150:PRO:HD3	2.07	0.53
1:B:1192:ASN:O	1:B:1196:GLU:HG3	2.08	0.53
1:D:1103:ASP:OD1	1:D:1106:GLU:HB2	2.08	0.53
2:H:501:GLU:OE1	2:H:552:LYS:HD3	2.09	0.53
1:C:3:ARG:NE	1:C:27:ASN:HD21	2.03	0.53
1:C:1083:THR:HG21	1:C:1095:GLY:HA3	1.89	0.53
1:A:95:LYS:HE2	1:A:108:MET:CE	2.39	0.53
1:B:158:ALA:HB1	1:B:1126:MET:HE2	1.91	0.53
2:H:511:GLN:O	2:H:512:ALA:HB2	2.08	0.53
1:B:1204:VAL:HG22	1:B:1215:ILE:CD1	2.38	0.53
1:B:98:TYR:CZ	1:B:138:GLU:HG2	2.43	0.53
2:E:511:GLN:O	2:E:512:ALA:HB2	2.08	0.53
1:C:3:ARG:HH21	1:C:3:ARG:HB2	1.74	0.52
2:G:506:ASP:O	2:G:509:LYS:HB3	2.09	0.52
1:A:142:ILE:N	1:A:142:ILE:CD1	2.71	0.52
1:D:53:ARG:HD3	1:D:54:SER:CB	2.40	0.52
1:A:119:TYR:HD2	1:A:131:TYR:CD2	2.27	0.52
2:E:496:LEU:HD13	2:E:555:ALA:CB	2.30	0.52
1:A:1216:ILE:HA	2:E:544:GLN:NE2	2.24	0.52
1:A:127:SER:O	1:A:128:TYR:C	2.46	0.52
1:C:1168:VAL:HG11	1:C:1193:THR:HB	1.90	0.52
1:D:1126:MET:HE3	1:D:1129:LEU:HD12	1.90	0.52
1:D:1141:LEU:HD22	1:D:1145:ILE:CD1	2.38	0.52
1:A:49:VAL:HG13	1:A:94:VAL:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:GLN:HG3	1:B:178:TYR:N	2.24	0.52
2:E:493:ARG:HE	2:E:560:PHE:HD2	1.56	0.52
1:C:1196:GLU:OE1	2:G:522:ARG:HG3	2.08	0.52
1:D:182:TYR:HD1	1:D:1056:ILE:HG22	1.75	0.52
1:A:1118:PRO:HD3	1:A:1129:LEU:HD21	1.92	0.52
1:B:49:VAL:HG13	1:B:94:VAL:CG1	2.39	0.52
1:C:10:SER:HA	1:C:17:GLY:O	2.10	0.52
1:D:1179:ARG:C	1:D:1179:ARG:HD2	2.30	0.52
2:F:492:LEU:HD13	2:F:540:ILE:HD11	1.91	0.52
1:D:2:GLY:HA3	1:D:98:TYR:CZ	2.45	0.52
1:B:1220:LEU:HB3	2:F:521:LYS:HE3	1.91	0.52
2:G:492:LEU:HD13	2:G:540:ILE:HD11	1.90	0.52
1:A:119:TYR:CD2	1:A:131:TYR:CD2	2.98	0.51
1:A:1207:GLN:NE2	1:A:1210:GLU:HB2	2.25	0.51
1:C:162:PRO:HB2	1:C:1111:GLY:HA3	1.93	0.51
1:B:168:MET:O	1:B:172:VAL:HG23	2.10	0.51
1:B:177:GLN:CG	1:B:178:TYR:N	2.73	0.51
1:B:97:PHE:HB3	1:B:104:LEU:HD21	1.90	0.51
1:B:1179:ARG:C	1:B:1179:ARG:HD2	2.31	0.51
2:G:531:ILE:CG2	2:G:542:LEU:HD21	2.40	0.51
1:C:1216:ILE:HD12	2:G:551:ILE:HD13	1.92	0.51
1:B:65:LEU:O	1:B:66:ILE:O	2.28	0.51
1:B:1205:TYR:HE2	1:B:1216:ILE:HG23	1.75	0.51
1:B:3:ARG:NH2	1:B:3:ARG:HB3	2.26	0.51
1:A:1081:GLU:C	1:A:1083:THR:H	2.14	0.51
1:A:1148:TYR:CD2	1:A:1149:GLN:HG3	2.45	0.51
1:B:165:LEU:HD22	1:B:169:PHE:CE1	2.45	0.51
1:C:97:PHE:HB3	1:C:104:LEU:HD21	1.92	0.51
1:A:3:ARG:NE	1:A:27:ASN:HD21	2.05	0.51
2:E:504:PHE:CD1	2:E:531:ILE:CD1	2.89	0.51
2:G:485:ILE:O	2:G:485:ILE:HG22	2.11	0.51
2:G:511:GLN:O	2:G:512:ALA:HB2	2.11	0.51
2:H:556:LYS:HB3	2:H:557:PRO:HD2	1.93	0.51
1:D:102:ASN:ND2	1:D:102:ASN:N	2.59	0.51
1:D:189:ILE:HD11	1:D:1049:ILE:HG23	1.92	0.51
1:B:1071:VAL:HG22	1:B:1145:ILE:HA	1.92	0.51
1:B:1216:ILE:HA	2:F:544:GLN:NE2	2.25	0.51
1:D:1050:LEU:O	1:D:1054:LEU:HG	2.11	0.51
1:D:1146:ASN:HD21	1:D:1151:SER:H	1.58	0.51
1:D:185:LEU:O	1:D:189:ILE:HD13	2.11	0.51
2:E:510:SER:O	2:E:511:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:493:ARG:HE	2:G:560:PHE:HD2	1.58	0.51
1:A:154:VAL:CG1	1:A:155:GLU:N	2.74	0.50
1:D:1148:TYR:O	1:D:1150:PRO:HD3	2.11	0.50
1:D:1160:ASP:OD2	1:D:1194:MET:HG3	2.10	0.50
2:F:556:LYS:HB3	2:F:557:PRO:HD2	1.93	0.50
1:A:158:ALA:HB1	1:A:1126:MET:HE2	1.93	0.50
1:A:141:LEU:C	1:A:143:LYS:H	2.15	0.50
1:B:1071:VAL:CG2	1:B:1145:ILE:HA	2.42	0.50
1:B:189:ILE:HD12	1:B:189:ILE:H	1.76	0.50
1:B:65:LEU:HD12	1:B:111:ILE:HD13	1.93	0.50
1:C:95:LYS:HE2	1:C:108:MET:CE	2.41	0.50
1:D:129:LYS:O	1:D:133:ILE:HG13	2.11	0.50
1:D:1217:THR:OG1	2:H:547:ALA:O	2.27	0.50
1:B:98:TYR:O	1:B:104:LEU:HD23	2.11	0.50
2:G:504:PHE:CD1	2:G:531:ILE:CD1	2.89	0.50
2:H:559:LEU:HD22	2:H:559:LEU:O	2.12	0.50
1:D:182:TYR:CE1	1:D:1057:LYS:HG3	2.47	0.50
1:A:1082:LEU:HD22	1:A:1171:ILE:HD13	1.93	0.50
1:A:95:LYS:HD3	1:A:106:GLU:OE1	2.12	0.50
1:A:50:LEU:HD22	1:A:140:ILE:HG21	1.92	0.50
1:B:16:ARG:HB2	1:B:67:TYR:CE1	2.46	0.50
1:C:1152:PRO:HG2	1:C:1153:PHE:CD2	2.47	0.50
1:C:4:LEU:N	1:C:1184:GLN:HE22	1.99	0.50
1:A:12:PHE:O	1:A:13:LYS:HG3	2.12	0.49
1:B:1101:ILE:HD13	1:B:1107:PRO:HB3	1.94	0.49
1:B:1141:LEU:HD22	1:B:1145:ILE:HD11	1.94	0.49
1:B:1218:LEU:HD23	1:B:1219:ASP:N	2.28	0.49
1:D:1180:ASN:OD1	1:D:1182:ASP:N	2.40	0.49
1:D:188:LYS:HD2	1:D:1049:ILE:HG12	1.93	0.49
1:C:1218:LEU:HD23	1:C:1219:ASP:N	2.27	0.49
1:D:53:ARG:C	1:D:53:ARG:CD	2.79	0.49
1:A:3:ARG:HH21	1:A:3:ARG:HB2	1.77	0.49
1:B:116:ASP:OD2	2:G:494:LYS:HE3	2.12	0.49
2:H:504:PHE:CD1	2:H:531:ILE:CD1	2.89	0.49
1:A:1153:PHE:HB3	1:A:1184:GLN:HB3	1.95	0.49
1:C:1053:PHE:C	1:C:1055:LYS:H	2.16	0.49
2:H:546:GLU:O	2:H:547:ALA:C	2.50	0.49
2:F:511:GLN:O	2:F:512:ALA:HB2	2.12	0.49
1:B:161:SER:OG	1:B:164:GLU:HG3	2.12	0.49
1:C:67:TYR:CZ	1:C:68:ARG:O	2.66	0.49
1:C:131:TYR:O	1:C:134:PHE:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1048:LYS:HD3	1:B:1048:LYS:O	2.13	0.49
1:B:43:MET:HG3	1:B:1155:VAL:CG1	2.41	0.49
1:C:1223:TYR:N	1:C:1223:TYR:CD1	2.80	0.49
1:A:1216:ILE:HG13	2:E:528:PHE:CZ	2.48	0.49
1:D:1060:ARG:HG2	1:D:1108:PHE:CE2	2.48	0.49
1:D:1080:ARG:HG2	1:D:1095:GLY:O	2.12	0.48
1:C:102:ASN:N	1:C:102:ASN:ND2	2.60	0.48
1:C:143:LYS:CG	1:C:171:GLU:HG3	2.40	0.48
1:D:158:ALA:HB1	1:D:1126:MET:HE2	1.94	0.48
1:D:95:LYS:HE2	1:D:108:MET:HE1	1.91	0.48
1:C:1064:PHE:C	1:C:1064:PHE:CD2	2.85	0.48
1:C:49:VAL:HG13	1:C:94:VAL:HB	1.94	0.48
2:H:496:LEU:CD1	2:H:555:ALA:HB2	2.24	0.48
1:A:1160:ASP:OD2	1:A:1194:MET:HG3	2.13	0.48
1:D:1217:THR:H	2:H:544:GLN:NE2	1.97	0.48
1:B:49:VAL:HG13	1:B:94:VAL:HB	1.95	0.48
1:C:1066:LYS:HE2	1:C:1148:TYR:OH	2.13	0.48
1:C:1160:ASP:OD2	1:C:1194:MET:HG3	2.13	0.48
1:C:138:GLU:O	1:C:139:ASN:HB2	2.13	0.48
1:B:62:LEU:O	1:B:65:LEU:HG	2.14	0.48
1:B:65:LEU:O	1:B:66:ILE:C	2.51	0.48
1:A:51:GLY:HA2	1:A:119:TYR:HE2	1.79	0.48
1:A:1205:TYR:HE2	1:A:1216:ILE:HG23	1.78	0.48
1:D:10:SER:HA	1:D:17:GLY:O	2.14	0.48
1:B:102:ASN:N	1:B:102:ASN:ND2	2.60	0.48
1:B:66:ILE:HD13	1:B:92:ALA:HB2	1.96	0.48
1:C:179:LYS:HD2	1:C:1060:ARG:NH1	2.29	0.48
1:C:98:TYR:CE2	1:C:138:GLU:HG2	2.49	0.48
1:C:1119:PRO:C	1:C:1121:LYS:H	2.17	0.47
1:C:175:SER:N	1:C:1063:LEU:HD13	2.29	0.47
1:A:1179:ARG:HD2	1:A:1179:ARG:O	2.13	0.47
1:C:1217:THR:H	2:G:544:GLN:NE2	1.99	0.47
1:A:141:LEU:O	1:A:141:LEU:HD23	2.15	0.47
1:A:39:LYS:O	1:A:42:MET:HB2	2.14	0.47
1:B:12:PHE:CE1	1:B:13:LYS:HG3	2.49	0.47
1:C:158:ALA:HB1	1:C:1126:MET:HE2	1.97	0.47
1:C:12:PHE:CD1	1:C:13:LYS:HG3	2.49	0.47
1:D:1119:PRO:C	1:D:1121:LYS:H	2.14	0.47
1:B:1208:GLN:NE2	2:F:538:GLY:HA3	2.28	0.47
1:A:1172:ALA:HB1	1:A:1197:LYS:HD2	1.96	0.47
1:D:174:GLY:C	1:D:176:ILE:H	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ARG:HD3	1:D:54:SER:HB3	1.95	0.47
2:F:546:GLU:O	2:F:547:ALA:C	2.53	0.47
1:A:98:TYR:HE2	1:A:138:GLU:OE1	1.97	0.47
1:C:49:VAL:CG1	1:C:94:VAL:HG12	2.45	0.47
1:B:30:SER:HA	1:B:1187:VAL:O	2.14	0.47
1:C:1216:ILE:HG13	2:G:528:PHE:CZ	2.50	0.47
1:D:1082:LEU:HD22	1:D:1171:ILE:HD13	1.96	0.47
1:D:1205:TYR:CZ	1:D:1214:LYS:HB2	2.50	0.47
1:D:98:TYR:CZ	1:D:138:GLU:HG2	2.50	0.47
2:E:492:LEU:HD21	2:E:507:VAL:HG21	1.95	0.47
1:D:1082:LEU:HD22	1:D:1171:ILE:CD1	2.44	0.47
1:D:146:ASN:HD22	1:D:146:ASN:N	2.11	0.47
1:D:189:ILE:CD1	1:D:189:ILE:N	2.73	0.47
1:C:179:LYS:CD	1:C:1060:ARG:NH1	2.77	0.47
1:D:26:SER:OG	1:D:1199:ASP:HB2	2.15	0.47
2:G:499:GLU:HG3	2:G:501:GLU:H	1.80	0.47
1:C:102:ASN:HD22	1:C:102:ASN:N	2.13	0.47
1:C:143:LYS:HG3	1:C:171:GLU:OE1	2.15	0.47
1:D:188:LYS:CD	1:D:1049:ILE:HG12	2.45	0.47
2:F:504:PHE:CD1	2:F:531:ILE:CD1	2.92	0.46
1:D:1216:ILE:HD13	2:H:542:LEU:HD13	1.97	0.46
2:E:556:LYS:HB3	2:E:557:PRO:HD2	1.95	0.46
1:B:154:VAL:HG13	1:B:155:GLU:N	2.29	0.46
1:A:141:LEU:HD23	1:A:143:LYS:H	1.79	0.46
1:D:1168:VAL:HG11	1:D:1193:THR:HB	1.96	0.46
1:D:178:TYR:CE1	1:D:1059:LYS:HG3	2.51	0.46
1:B:49:VAL:CG1	1:B:94:VAL:HG12	2.46	0.46
1:B:179:LYS:O	1:B:183:GLU:HG2	2.15	0.46
1:D:30:SER:HA	1:D:1187:VAL:O	2.16	0.46
1:D:1206:ARG:NH2	1:D:1206:ARG:CG	2.76	0.46
2:G:492:LEU:HD13	2:G:540:ILE:HD12	1.98	0.46
1:A:146:ASN:N	1:A:146:ASN:ND2	2.61	0.46
1:A:97:PHE:HB3	1:A:104:LEU:HD21	1.98	0.46
1:D:65:LEU:O	1:D:66:ILE:HB	2.15	0.46
1:C:31:ILE:HB	1:C:1188:ILE:HG12	1.98	0.46
1:D:49:VAL:HG13	1:D:94:VAL:HB	1.98	0.46
1:A:98:TYR:O	1:A:104:LEU:HD23	2.16	0.45
1:A:10:SER:CB	1:A:93:TYR:CE1	2.99	0.45
1:B:1168:VAL:HG13	1:B:1194:MET:HG2	1.97	0.45
1:C:1205:TYR:CZ	1:C:1214:LYS:HB2	2.51	0.45
1:D:114:ASN:ND2	1:D:116:ASP:HB2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:485:ILE:HG22	2:E:485:ILE:O	2.15	0.45
1:B:68:ARG:HG3	1:B:68:ARG:NH2	2.31	0.45
1:B:1217:THR:OG1	2:F:547:ALA:O	2.35	0.45
1:A:125:THR:HG22	1:A:126:VAL:N	2.32	0.45
1:B:1119:PRO:C	1:B:1121:LYS:H	2.19	0.45
1:B:54:SER:CA	1:B:145:LYS:NZ	2.74	0.45
1:B:160:GLN:HE22	1:B:168:MET:HE1	1.82	0.45
1:D:16:ARG:HD2	1:D:67:TYR:CZ	2.50	0.45
1:C:120:LYS:HG2	1:C:125:THR:HA	1.98	0.45
1:C:3:ARG:CB	1:C:3:ARG:NH2	2.79	0.45
1:D:1179:ARG:NH2	1:D:1199:ASP:OD2	2.50	0.45
1:B:1049:ILE:HD12	1:B:1052:GLN:OE1	2.16	0.45
1:B:1207:GLN:NE2	1:B:1210:GLU:HB2	2.31	0.45
1:A:100:LYS:CE	1:A:138:GLU:OE2	2.64	0.45
2:E:546:GLU:O	2:E:547:ALA:C	2.54	0.45
1:B:1206:ARG:HH21	1:B:1206:ARG:CG	2.29	0.45
1:C:95:LYS:HE2	1:C:108:MET:HE2	1.98	0.45
1:A:12:PHE:CD1	1:A:45:ALA:HB2	2.51	0.45
1:A:49:VAL:CG1	1:A:94:VAL:HG12	2.47	0.45
1:B:3:ARG:HH21	1:B:3:ARG:CB	2.30	0.45
1:C:1056:ILE:HG22	1:C:1057:LYS:N	2.32	0.45
1:C:146:ASN:N	1:C:146:ASN:HD22	2.09	0.45
2:H:492:LEU:HD21	2:H:507:VAL:HG21	1.99	0.45
1:B:1060:ARG:NH2	1:B:1108:PHE:CD1	2.86	0.44
1:C:1083:THR:C	1:C:1170:ARG:NH2	2.70	0.44
1:D:1060:ARG:HG2	1:D:1108:PHE:CD2	2.52	0.44
1:D:1157:ASP:O	1:D:1188:ILE:O	2.35	0.44
1:C:1196:GLU:HG2	2:G:522:ARG:HA	1.99	0.44
1:A:65:LEU:HD12	1:A:111:ILE:HD13	2.00	0.44
1:A:49:VAL:C	1:A:51:GLY:H	2.19	0.44
1:B:129:LYS:HA	2:G:500:LYS:HG2	2.00	0.44
1:C:1214:LYS:O	1:C:1215:ILE:HD13	2.16	0.44
1:D:1071:VAL:CG2	1:D:1145:ILE:HA	2.48	0.44
1:D:154:VAL:CG1	1:D:155:GLU:N	2.80	0.44
2:H:485:ILE:HG22	2:H:485:ILE:O	2.18	0.44
2:F:540:ILE:HG23	2:F:541:GLY:N	2.33	0.44
1:B:1083:THR:HG23	1:B:1119:PRO:HG3	1.99	0.44
2:E:504:PHE:HD1	2:E:531:ILE:HD11	1.72	0.44
2:E:559:LEU:O	2:E:559:LEU:HD22	2.17	0.44
1:C:1064:PHE:CE2	1:C:1107:PRO:HB2	2.52	0.44
1:A:30:SER:HA	1:A:1187:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:VAL:HG11	1:A:1194:MET:CE	2.48	0.44
1:A:160:GLN:HE22	1:A:168:MET:CE	2.30	0.44
1:C:129:LYS:O	1:C:133:ILE:HG13	2.17	0.44
1:C:147:PHE:CE1	1:C:148:LEU:HG	2.53	0.44
1:D:1192:ASN:O	1:D:1196:GLU:HG3	2.17	0.44
1:D:143:LYS:HG2	1:D:171:GLU:CG	2.48	0.44
1:B:138:GLU:O	1:B:139:ASN:HB2	2.16	0.44
1:B:16:ARG:HB3	1:B:1212:SER:HB2	2.00	0.44
1:B:66:ILE:CD1	1:B:92:ALA:N	2.80	0.44
1:D:4:LEU:H	1:D:1184:GLN:NE2	1.95	0.44
2:F:493:ARG:HE	2:F:560:PHE:HD2	1.66	0.44
1:A:131:TYR:HE2	1:A:135:LEU:HD11	1.83	0.44
1:A:158:ALA:HB1	1:A:1126:MET:CE	2.48	0.44
1:A:8:GLU:HB3	1:A:95:LYS:HB2	1.99	0.44
1:B:1080:ARG:HG2	1:B:1095:GLY:O	2.17	0.44
1:C:173:SER:HB2	1:C:1063:LEU:HD22	2.00	0.44
1:A:1083:THR:CG2	1:A:1119:PRO:HD3	2.44	0.43
1:B:1167:ASN:HA	1:B:1170:ARG:HG3	1.99	0.43
1:B:158:ALA:HB1	1:B:1126:MET:HE1	2.00	0.43
1:A:138:GLU:O	1:A:140:ILE:HG13	2.17	0.43
1:B:1168:VAL:HG11	1:B:1193:THR:HB	1.99	0.43
1:B:16:ARG:HD2	1:B:67:TYR:CZ	2.52	0.43
1:C:177:GLN:HG3	1:C:178:TYR:CD1	2.54	0.43
1:D:1148:TYR:C	1:D:1150:PRO:HD3	2.38	0.43
1:D:1218:LEU:HD23	1:D:1219:ASP:N	2.33	0.43
2:G:559:LEU:HD22	2:G:559:LEU:O	2.18	0.43
1:D:114:ASN:HD21	1:D:116:ASP:HB2	1.83	0.43
1:D:11:ASN:O	1:D:66:ILE:HA	2.19	0.43
1:A:52:VAL:HG23	1:A:142:ILE:HB	1.96	0.43
1:D:47:SER:O	1:D:51:GLY:O	2.36	0.43
2:F:485:ILE:HG22	2:F:485:ILE:O	2.18	0.43
1:A:1179:ARG:NH2	1:A:1199:ASP:OD2	2.52	0.43
4:A:2224:AGS:O2'	1:B:1121:LYS:HD3	2.18	0.43
1:B:1148:TYR:O	1:B:1150:PRO:HD3	2.19	0.43
1:A:141:LEU:CD2	1:A:143:LYS:HB3	2.49	0.43
1:A:10:SER:HB2	1:A:93:TYR:CE1	2.53	0.43
1:B:1196:GLU:OE1	2:F:522:ARG:HG3	2.18	0.43
1:B:3:ARG:NH2	1:B:3:ARG:CB	2.82	0.43
1:B:10:SER:HB2	1:B:93:TYR:CE1	2.53	0.43
1:C:1179:ARG:O	1:C:1179:ARG:HD2	2.19	0.43
2:F:492:LEU:HD21	2:F:507:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ILE:HG21	1:D:1195:PHE:CD2	2.53	0.43
2:G:556:LYS:HB3	2:G:557:PRO:HD2	2.00	0.43
1:A:1218:LEU:HD23	1:A:1219:ASP:N	2.34	0.43
4:A:2224:AGS:O3'	1:B:1121:LYS:HE3	2.19	0.43
1:C:16:ARG:HD2	1:C:67:TYR:CZ	2.53	0.43
1:D:1218:LEU:CD2	1:D:1219:ASP:N	2.82	0.43
1:D:2:GLY:O	1:D:1152:PRO:HB2	2.18	0.43
2:E:559:LEU:O	2:E:559:LEU:CD2	2.67	0.43
1:C:37:SER:HA	1:C:1206:ARG:HG2	2.01	0.43
1:A:1183:LEU:HD13	1:A:1185:PHE:HE1	1.82	0.42
1:B:1134:LYS:HE3	1:B:1134:LYS:HB2	1.86	0.42
1:B:1183:LEU:HD13	1:B:1185:PHE:HE1	1.80	0.42
1:A:141:LEU:O	1:A:141:LEU:CD2	2.67	0.42
2:G:540:ILE:HD13	2:G:553:ILE:CG2	2.49	0.42
1:C:1126:MET:HE3	1:C:1129:LEU:HD12	2.01	0.42
1:A:27:ASN:HD22	1:A:27:ASN:HA	1.65	0.42
1:A:2:GLY:HA2	1:A:99:GLN:O	2.20	0.42
1:C:1082:LEU:HD22	1:C:1171:ILE:CD1	2.50	0.42
1:D:1048:LYS:C	1:D:1050:LEU:N	2.72	0.42
1:D:8:GLU:HB3	1:D:95:LYS:HB2	2.01	0.42
1:C:4:LEU:H	1:C:1184:GLN:NE2	2.00	0.42
1:D:170:GLU:HG2	1:D:175:SER:O	2.20	0.42
2:G:540:ILE:HG23	2:G:541:GLY:N	2.34	0.42
1:B:1083:THR:C	1:B:1170:ARG:NH2	2.73	0.42
1:C:1180:ASN:OD1	1:C:1182:ASP:N	2.41	0.42
1:C:30:SER:HA	1:C:1187:VAL:O	2.20	0.42
1:C:154:VAL:HG13	1:C:155:GLU:N	2.34	0.42
1:D:98:TYR:O	1:D:104:LEU:HD23	2.20	0.42
1:A:1148:TYR:C	1:A:1150:PRO:HD3	2.40	0.42
1:A:1216:ILE:HD13	2:E:542:LEU:HD13	2.01	0.42
1:A:165:LEU:HD23	1:A:165:LEU:O	2.19	0.42
1:C:1079:TYR:CD2	1:C:1097:ALA:HB2	2.54	0.42
1:C:173:SER:O	1:C:1063:LEU:HD21	2.20	0.42
1:A:3:ARG:CB	1:A:3:ARG:NH2	2.82	0.41
1:B:108:MET:HG2	1:B:109:ARG:N	2.35	0.41
1:B:177:GLN:CG	1:B:178:TYR:H	2.33	0.41
1:B:98:TYR:OH	1:B:138:GLU:CG	2.68	0.41
1:A:49:VAL:HG13	1:A:94:VAL:CB	2.50	0.41
1:B:179:LYS:HD3	1:B:1060:ARG:HH12	1.79	0.41
1:C:162:PRO:O	1:C:1111:GLY:HA2	2.20	0.41
1:C:174:GLY:O	1:C:177:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:GLY:O	1:D:176:ILE:N	2.48	0.41
2:F:496:LEU:HD13	2:F:555:ALA:CB	2.33	0.41
1:A:110:ILE:O	1:A:117:THR:HA	2.20	0.41
1:A:100:LYS:NZ	1:A:138:GLU:OE2	2.51	0.41
2:E:523:GLU:H	2:E:523:GLU:HG3	1.68	0.41
1:C:1192:ASN:ND2	2:G:526:ARG:HD2	2.35	0.41
1:A:1119:PRO:C	1:A:1121:LYS:H	2.22	0.41
1:A:1168:VAL:HG13	1:A:1194:MET:HG2	2.03	0.41
1:B:1048:LYS:HD3	1:B:1048:LYS:C	2.41	0.41
1:B:146:ASN:HD22	1:B:146:ASN:N	2.17	0.41
1:C:1125:ASP:O	1:C:1127:GLU:N	2.54	0.41
1:C:93:TYR:CD2	1:C:93:TYR:C	2.93	0.41
2:E:540:ILE:HG23	2:E:541:GLY:N	2.35	0.41
2:H:531:ILE:HD13	2:H:531:ILE:HG21	1.80	0.41
1:D:98:TYR:OH	1:D:138:GLU:CG	2.69	0.41
1:B:10:SER:CB	1:B:93:TYR:CE1	3.03	0.41
1:C:34:PRO:HG2	1:C:37:SER:HB3	2.02	0.41
1:D:183:GLU:O	1:D:187:GLU:HB2	2.21	0.41
1:A:1205:TYR:CE1	1:A:1214:LYS:HB2	2.55	0.41
1:A:140:ILE:O	1:A:142:ILE:N	2.53	0.41
1:A:15:TYR:OH	1:A:42:MET:HG2	2.21	0.41
1:B:170:GLU:OE1	1:B:1060:ARG:NE	2.52	0.41
1:C:1049:ILE:C	1:C:1051:ASN:H	2.23	0.41
1:A:31:ILE:HB	1:A:1188:ILE:HG12	2.01	0.41
1:C:1109:ASN:HA	1:C:1109:ASN:HD22	1.61	0.41
1:C:16:ARG:HB3	1:C:1212:SER:HB2	2.01	0.41
1:C:16:ARG:HB2	1:C:67:TYR:CE1	2.56	0.41
1:A:1220:LEU:HB3	2:E:521:LYS:HE3	2.02	0.41
2:F:559:LEU:CD2	2:F:559:LEU:O	2.69	0.41
1:A:1223:TYR:CD1	1:A:1223:TYR:N	2.88	0.41
1:D:178:TYR:C	1:D:180:LYS:N	2.74	0.41
1:D:188:LYS:HB2	1:D:189:ILE:HD12	2.02	0.41
1:A:142:ILE:HG23	1:A:147:PHE:CZ	2.56	0.41
1:B:109:ARG:NH1	1:B:117:THR:HG21	2.32	0.41
1:B:16:ARG:HD2	1:B:67:TYR:OH	2.21	0.41
1:C:174:GLY:C	1:C:176:ILE:N	2.75	0.41
1:D:100:LYS:HE3	1:D:138:GLU:OE1	2.21	0.41
1:D:1101:ILE:CG2	1:D:1107:PRO:HB3	2.50	0.41
1:D:166:SER:HB2	1:D:1111:GLY:HA2	2.02	0.41
1:D:1174:TYR:C	1:D:1174:TYR:CD2	2.94	0.41
1:D:1183:LEU:HA	1:D:1183:LEU:HD23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1196:GLU:OE1	2:G:522:ARG:NE	2.54	0.41
1:C:1201:LEU:HD11	2:G:525:SER:HB3	2.02	0.41
2:H:493:ARG:HE	2:H:560:PHE:HD2	1.69	0.41
1:A:1125:ASP:C	1:A:1127:GLU:N	2.73	0.41
1:A:1192:ASN:O	1:A:1196:GLU:HG3	2.21	0.41
1:A:34:PRO:HG2	1:A:37:SER:HB3	2.03	0.41
1:B:68:ARG:CG	1:B:68:ARG:HH21	2.33	0.41
1:D:1067:THR:HG23	1:D:1148:TYR:CD2	2.56	0.41
1:D:41:ASN:O	1:D:44:ASP:HB2	2.21	0.41
1:C:1172:ALA:HB1	1:C:1197:LYS:HD2	2.03	0.40
1:D:10:SER:CB	1:D:93:TYR:CE1	3.05	0.40
1:A:1196:GLU:OE1	2:E:522:ARG:HG3	2.21	0.40
1:A:10:SER:HB2	1:A:93:TYR:CZ	2.56	0.40
1:B:1081:GLU:OE1	1:B:1177:ARG:HD3	2.21	0.40
1:B:1205:TYR:CZ	1:B:1214:LYS:HB2	2.57	0.40
1:C:10:SER:HB3	1:C:93:TYR:CD1	2.56	0.40
2:G:499:GLU:HG3	2:G:500:LYS:N	2.35	0.40
1:B:127:SER:HB3	2:G:560:PHE:HE1	1.86	0.40
1:B:1123:PHE:HD2	1:B:1123:PHE:HA	1.81	0.40
1:D:62:LEU:HD23	1:D:62:LEU:HA	1.90	0.40
2:E:540:ILE:HD13	2:E:553:ILE:CG2	2.51	0.40
1:A:167:ARG:O	1:A:167:ARG:HD3	2.21	0.40
1:D:1118:PRO:O	1:D:1119:PRO:O	2.40	0.40
2:G:523:GLU:H	2:G:523:GLU:HG3	1.76	0.40
1:A:1180:ASN:OD1	1:A:1182:ASP:N	2.45	0.40
1:A:51:GLY:O	1:A:128:TYR:OH	2.30	0.40
1:D:27:ASN:HD22	1:D:27:ASN:HA	1.69	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	262/430 (61%)	233 (89%)	24 (9%)	5 (2%)	8 28
1	B	317/430 (74%)	288 (91%)	23 (7%)	6 (2%)	8 28
1	C	317/430 (74%)	284 (90%)	26 (8%)	7 (2%)	6 24
1	D	317/430 (74%)	283 (89%)	26 (8%)	8 (2%)	5 21
2	E	67/121 (55%)	62 (92%)	4 (6%)	1 (2%)	10 34
2	F	67/121 (55%)	63 (94%)	2 (3%)	2 (3%)	4 17
2	G	67/121 (55%)	62 (92%)	3 (4%)	2 (3%)	4 17
2	H	67/121 (55%)	62 (92%)	3 (4%)	2 (3%)	4 17
All	All	1481/2204 (67%)	1337 (90%)	111 (8%)	33 (2%)	6 24

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1119	PRO
1	A	1120	LEU
1	B	66	ILE
1	B	1119	PRO
1	B	1120	LEU
1	C	66	ILE
1	C	1119	PRO
1	C	1120	LEU
1	D	1119	PRO
1	D	1120	LEU
2	E	547	ALA
2	F	547	ALA
2	H	547	ALA
1	A	1157	ASP
1	B	1157	ASP
1	C	1157	ASP
1	D	67	TYR
1	D	1157	ASP
2	G	547	ALA
1	B	52	VAL
1	A	141	LEU
1	B	146	ASN
1	C	65	LEU
1	D	175	SER
2	H	511	GLN
1	A	142	ILE
1	C	1054	LEU

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Mol	Chain	Res	Type
1	C	1126	MET
1	D	52	VAL
1	D	66	ILE
2	F	511	GLN
2	G	511	GLN
1	D	1049	ILE

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	238/377 (63%)	220 (92%)	18 (8%)	13	36
1	B	288/377 (76%)	264 (92%)	24 (8%)	11	32
1	C	288/377 (76%)	263 (91%)	25 (9%)	10	30
1	D	288/377 (76%)	266 (92%)	22 (8%)	13	36
2	E	58/106 (55%)	53 (91%)	5 (9%)	10	30
2	F	58/106 (55%)	54 (93%)	4 (7%)	15	41
2	G	58/106 (55%)	54 (93%)	4 (7%)	15	41
2	H	58/106 (55%)	54 (93%)	4 (7%)	15	41
All	All	1334/1932 (69%)	1228 (92%)	106 (8%)	12	34

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	28	PHE
1	A	49	VAL
1	A	68	ARG
1	A	104	LEU
1	A	111	ILE
1	A	114	ASN
1	A	128	TYR
1	A	142	ILE

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Mol	Chain	Res	Type
1	A	146	ASN
1	A	165	LEU
1	A	1123	PHE
1	A	1141	LEU
1	A	1179	ARG
1	A	1183	LEU
1	A	1206	ARG
1	A	1207	GLN
1	A	1218	LEU
1	B	4	LEU
1	B	28	PHE
1	B	42	MET
1	B	53	ARG
1	B	68	ARG
1	B	104	LEU
1	B	111	ILE
1	B	114	ASN
1	B	138	GLU
1	B	146	ASN
1	B	165	LEU
1	B	1050	LEU
1	B	1056	ILE
1	B	1063	LEU
1	B	1075	LEU
1	B	1104	GLU
1	B	1123	PHE
1	B	1141	LEU
1	B	1179	ARG
1	B	1183	LEU
1	B	1206	ARG
1	B	1207	GLN
1	B	1217	THR
1	B	1218	LEU
1	C	4	LEU
1	C	28	PHE
1	C	42	MET
1	C	49	VAL
1	C	66	ILE
1	C	68	ARG
1	C	104	LEU
1	C	111	ILE
1	C	114	ASN

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Mol	Chain	Res	Type
1	C	138	GLU
1	C	146	ASN
1	C	165	LEU
1	C	1049	ILE
1	C	1056	ILE
1	C	1063	LEU
1	C	1075	LEU
1	C	1109	ASN
1	C	1123	PHE
1	C	1141	LEU
1	C	1179	ARG
1	C	1183	LEU
1	C	1194	MET
1	C	1206	ARG
1	C	1217	THR
1	C	1218	LEU
1	D	4	LEU
1	D	28	PHE
1	D	42	MET
1	D	49	VAL
1	D	53	ARG
1	D	102	ASN
1	D	104	LEU
1	D	111	ILE
1	D	114	ASN
1	D	129	LYS
1	D	146	ASN
1	D	165	LEU
1	D	1056	ILE
1	D	1063	LEU
1	D	1075	LEU
1	D	1123	PHE
1	D	1141	LEU
1	D	1179	ARG
1	D	1183	LEU
1	D	1206	ARG
1	D	1217	THR
1	D	1218	LEU
2	E	487	GLN
2	E	503	ILE
2	E	523	GLU
2	E	540	ILE

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Mol	Chain	Res	Type
2	E	559	LEU
2	F	487	GLN
2	F	525	SER
2	F	540	ILE
2	F	559	LEU
2	G	487	GLN
2	G	503	ILE
2	G	540	ILE
2	G	559	LEU
2	H	487	GLN
2	H	503	ILE
2	H	540	ILE
2	H	559	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	102	ASN
1	A	114	ASN
1	A	137	ASN
1	A	139	ASN
1	A	146	ASN
1	A	1149	GLN
1	A	1167	ASN
1	A	1184	GLN
1	A	1192	ASN
1	A	1208	GLN
1	A	1222	ASN
1	B	27	ASN
1	B	102	ASN
1	B	114	ASN
1	B	137	ASN
1	B	139	ASN
1	B	146	ASN
1	B	160	GLN
1	B	1109	ASN
1	B	1146	ASN
1	B	1149	GLN
1	B	1167	ASN
1	B	1184	GLN
1	B	1192	ASN

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Mol	Chain	Res	Type
1	B	1208	GLN
1	B	1222	ASN
1	C	27	ASN
1	C	102	ASN
1	C	114	ASN
1	C	137	ASN
1	C	139	ASN
1	C	146	ASN
1	C	177	GLN
1	C	1052	GLN
1	C	1109	ASN
1	C	1149	GLN
1	C	1167	ASN
1	C	1184	GLN
1	C	1192	ASN
1	C	1222	ASN
1	D	27	ASN
1	D	102	ASN
1	D	114	ASN
1	D	137	ASN
1	D	139	ASN
1	D	146	ASN
1	D	1052	GLN
1	D	1109	ASN
1	D	1146	ASN
1	D	1149	GLN
1	D	1167	ASN
1	D	1184	GLN
1	D	1192	ASN
1	D	1208	GLN
1	D	1222	ASN
2	E	487	GLN
2	E	544	GLN
2	E	550	ASN
2	F	487	GLN
2	F	544	GLN
2	F	550	ASN
2	G	487	GLN
2	G	544	GLN
2	G	550	ASN
2	H	487	GLN
2	H	544	GLN

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Mol	Chain	Res	Type
2	H	550	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	AGS	C	2224	3	26,33,33	1.71	7 (26%)	26,52,52	1.20	2 (7%)
4	AGS	A	2224	3	26,33,33	1.75	7 (26%)	26,52,52	1.31	2 (7%)
4	AGS	D	2224	3	26,33,33	1.72	7 (26%)	26,52,52	1.14	1 (3%)
4	AGS	B	2224	3	26,33,33	1.69	6 (23%)	26,52,52	1.21	2 (7%)

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
4	AGS	C	2224	3	-	4/17/38/38	0/3/3/3
4	AGS	A	2224	3	-	4/17/38/38	0/3/3/3
4	AGS	D	2224	3	-	7/17/38/38	0/3/3/3
4	AGS	B	2224	3	-	5/17/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2224	AGS	PG-S1G	-4.17	1.81	1.90
4	A	2224	AGS	PG-S1G	-4.15	1.81	1.90
4	C	2224	AGS	PG-S1G	-3.74	1.82	1.90
4	B	2224	AGS	C4-N3	3.63	1.40	1.35
4	A	2224	AGS	C4-N3	3.50	1.40	1.35
4	B	2224	AGS	PG-S1G	-3.46	1.83	1.90
4	C	2224	AGS	C4-N3	3.37	1.40	1.35
4	D	2224	AGS	C4-N3	3.34	1.40	1.35
4	A	2224	AGS	C6-N6	3.25	1.45	1.34
4	D	2224	AGS	C6-N6	3.16	1.45	1.34
4	C	2224	AGS	C2-N3	3.09	1.37	1.32
4	B	2224	AGS	C2-N3	3.08	1.37	1.32
4	C	2224	AGS	C6-N6	3.07	1.45	1.34
4	B	2224	AGS	C6-N6	2.98	1.44	1.34
4	D	2224	AGS	C2-N1	2.82	1.39	1.33
4	C	2224	AGS	C2-N1	2.77	1.39	1.33
4	B	2224	AGS	C2-N1	2.74	1.39	1.33
4	D	2224	AGS	C2-N3	2.71	1.36	1.32
4	C	2224	AGS	O4'-C4'	-2.65	1.39	1.45
4	A	2224	AGS	C2-N1	2.62	1.38	1.33
4	D	2224	AGS	O4'-C4'	-2.52	1.39	1.45
4	A	2224	AGS	O4'-C4'	-2.44	1.39	1.45
4	B	2224	AGS	O4'-C4'	-2.37	1.39	1.45
4	C	2224	AGS	PG-O2G	-2.33	1.47	1.54
4	A	2224	AGS	PG-O2G	-2.32	1.47	1.54
4	A	2224	AGS	C2-N3	2.21	1.35	1.32
4	D	2224	AGS	PG-O2G	-2.17	1.47	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2224	AGS	C4-C5-N7	3.12	112.65	109.40
4	C	2224	AGS	C4-C5-N7	2.81	112.33	109.40
4	D	2224	AGS	C4-C5-N7	2.59	112.10	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2224	AGS	C4-C5-N7	2.58	112.08	109.40
4	C	2224	AGS	O2A-PA-O1A	2.05	122.39	112.24
4	B	2224	AGS	O2A-PA-O1A	2.05	122.38	112.24
4	A	2224	AGS	O2G-PG-O3B	-2.02	97.91	104.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2224	AGS	C5'-O5'-PA-O2A
4	C	2224	AGS	C5'-O5'-PA-O1A
4	C	2224	AGS	C5'-O5'-PA-O2A
4	B	2224	AGS	C5'-O5'-PA-O2A
4	D	2224	AGS	C5'-O5'-PA-O2A
4	C	2224	AGS	C5'-O5'-PA-O3A
4	B	2224	AGS	C5'-O5'-PA-O3A
4	D	2224	AGS	C5'-O5'-PA-O3A
4	A	2224	AGS	PA-O3A-PB-O2B
4	D	2224	AGS	PA-O3A-PB-O2B
4	B	2224	AGS	C5'-O5'-PA-O1A
4	D	2224	AGS	C5'-O5'-PA-O1A
4	C	2224	AGS	PA-O3A-PB-O2B
4	D	2224	AGS	PG-O3B-PB-O2B
4	B	2224	AGS	PA-O3A-PB-O1B
4	B	2224	AGS	PA-O3A-PB-O2B
4	A	2224	AGS	PG-O3B-PB-O1B
4	A	2224	AGS	PG-O3B-PB-O2B
4	D	2224	AGS	PG-O3B-PB-O1B
4	D	2224	AGS	PA-O3A-PB-O1B

There are no ring outliers.

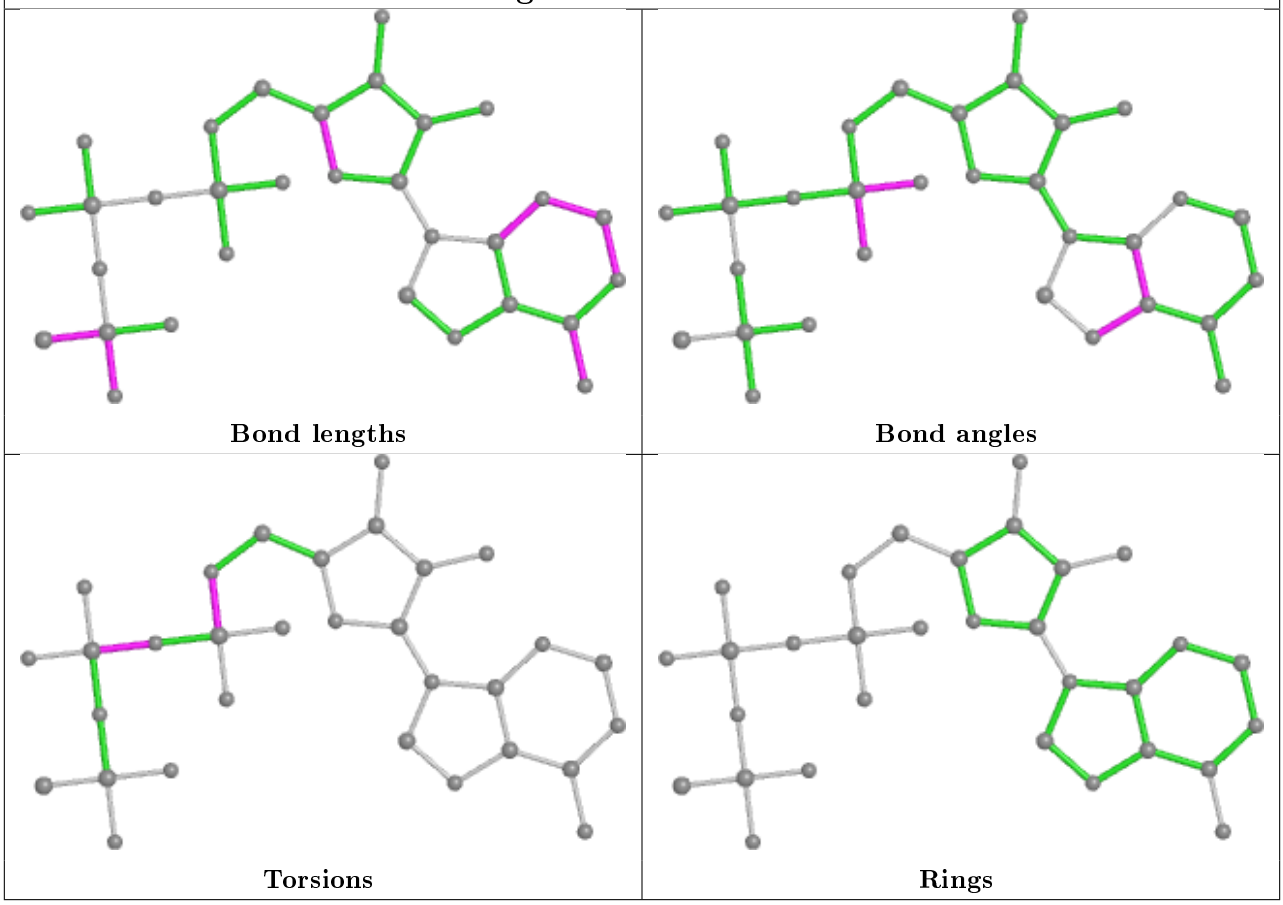
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2224	AGS	1	0
4	A	2224	AGS	3	0
4	D	2224	AGS	1	0

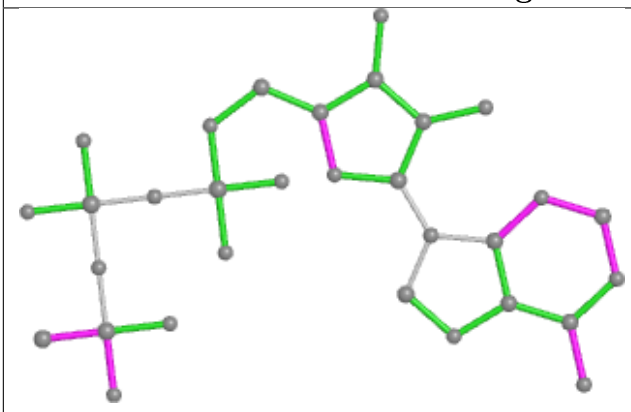
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

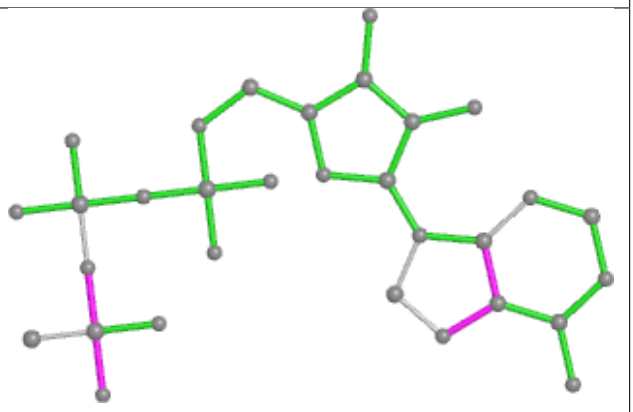
Ligand AGS C 2224



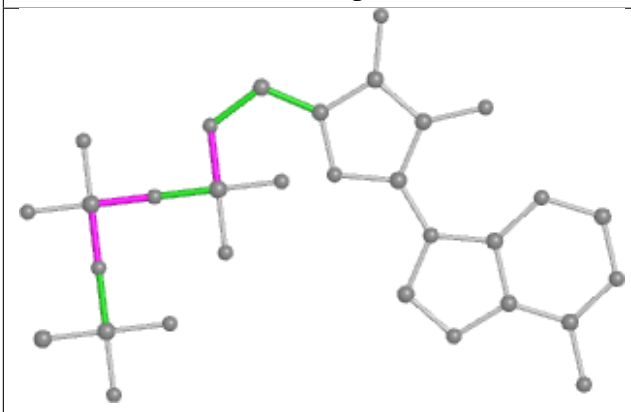
Ligand AGS A 2224



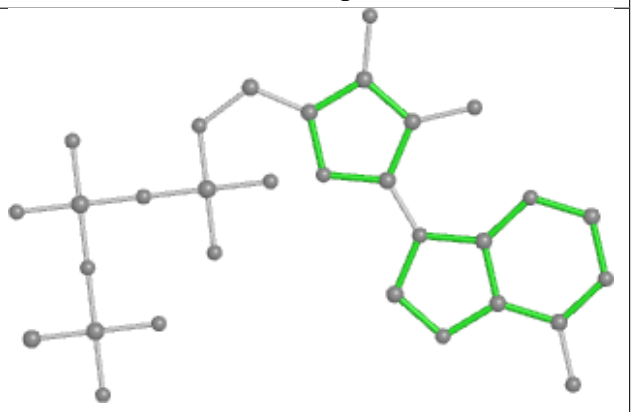
Bond lengths



Bond angles

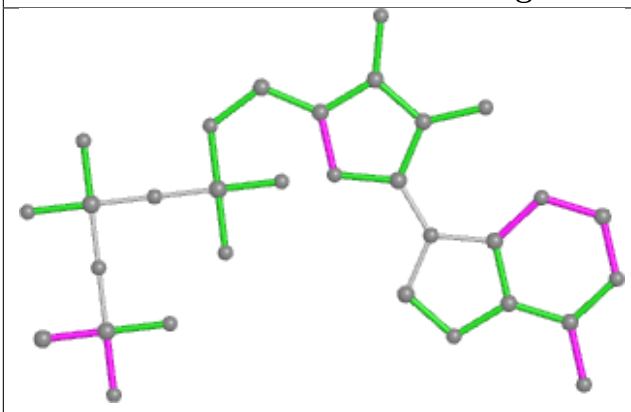


Torsions

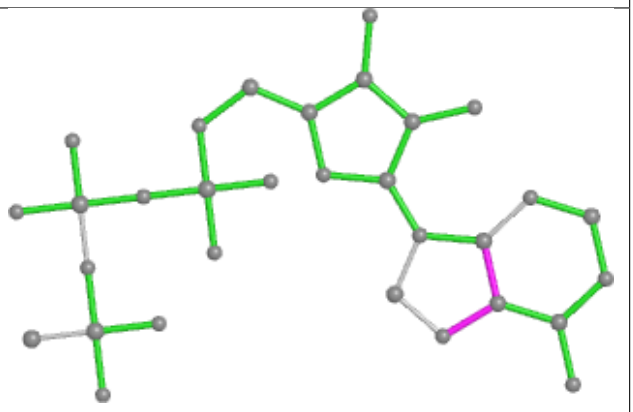


Rings

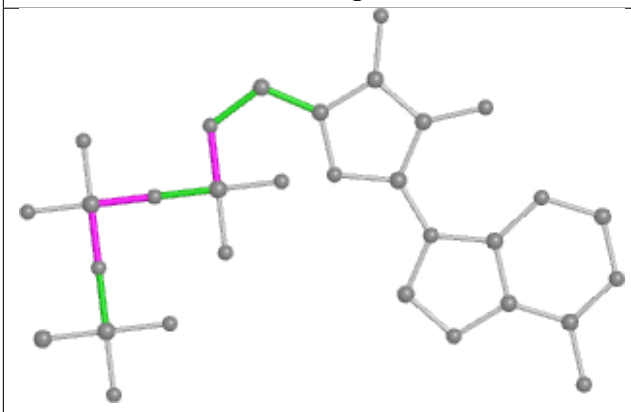
Ligand AGS D 2224



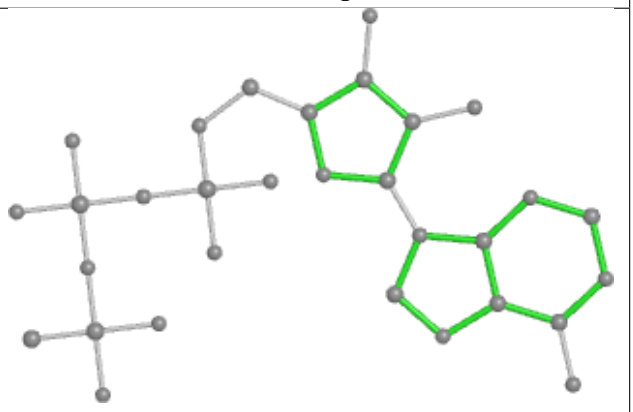
Bond lengths



Bond angles

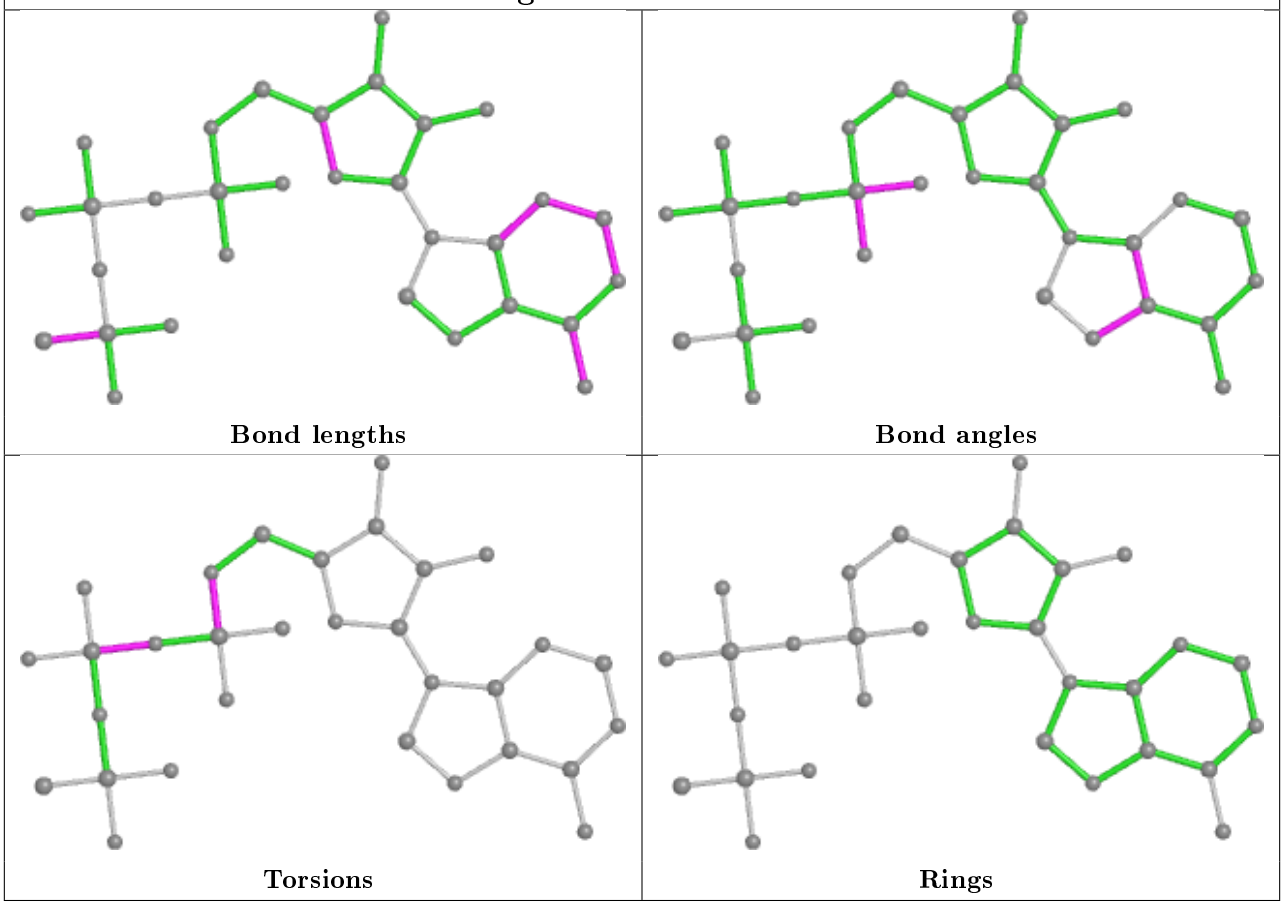


Torsions



Rings

Ligand AGS B 2224



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^{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	274/430 (63%)	1.00	37 (13%) 3 2	35, 64, 126, 158	0
1	B	327/430 (76%)	0.72	21 (6%) 19 15	31, 56, 96, 116	0
1	C	327/430 (76%)	0.61	11 (3%) 45 40	28, 52, 95, 110	0
1	D	327/430 (76%)	0.84	31 (9%) 8 6	25, 58, 110, 125	0
2	E	71/121 (58%)	1.18	11 (15%) 2 1	53, 85, 122, 131	0
2	F	71/121 (58%)	0.87	7 (9%) 7 5	53, 81, 112, 118	0
2	G	71/121 (58%)	0.65	2 (2%) 53 49	44, 66, 91, 100	0
2	H	71/121 (58%)	0.76	2 (2%) 53 49	41, 72, 101, 108	0
All	All	1539/2204 (69%)	0.80	122 (7%) 12 10	25, 61, 108, 158	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	VAL	11.9
1	D	100	LYS	8.0
2	F	485	ILE	7.7
2	E	485	ILE	6.9
1	D	1128	TYR	6.5
1	D	103	LYS	6.0
1	A	168	MET	5.7
1	D	1052	GLN	5.5
1	D	1124	LYS	5.2
1	A	1068	PHE	5.1
1	A	1126	MET	5.0
1	D	115	GLY	4.8
1	D	102	ASN	4.7
1	A	1067	THR	4.7
1	A	158	ALA	4.4
1	B	1052	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
2	E	498	GLU	4.3
1	A	1099	LEU	4.3
1	B	62	LEU	4.2
1	D	1123	PHE	4.1
1	A	1071	VAL	4.1
1	C	62	LEU	4.0
2	F	498	GLU	3.9
1	D	62	LEU	3.9
2	E	553	ILE	3.7
2	F	504	PHE	3.7
1	C	1120	LEU	3.7
1	A	62	LEU	3.6
1	B	113	ARG	3.4
1	A	1123	PHE	3.4
1	D	113	ARG	3.4
1	B	142	ILE	3.4
1	A	141	LEU	3.3
1	A	1122	ARG	3.2
2	F	509	LYS	3.2
1	D	1126	MET	3.2
1	B	1123	PHE	3.1
1	D	186	LYS	3.1
1	B	1122	ARG	3.0
1	D	1112	ILE	3.0
2	E	492	LEU	2.9
2	E	496	LEU	2.9
1	A	105	VAL	2.9
2	E	547	ALA	2.8
1	A	2	GLY	2.8
1	A	157	ILE	2.8
1	B	111	ILE	2.8
1	A	119	TYR	2.7
2	F	508	LEU	2.7
2	E	484	ALA	2.7
1	D	1055	LYS	2.7
2	E	531	ILE	2.7
1	A	63	LYS	2.6
1	C	1122	ARG	2.6
2	E	504	PHE	2.6
1	A	155	GLU	2.6
1	D	1054	LEU	2.5
1	B	115	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	101	GLY	2.5
1	A	165	LEU	2.5
1	C	113	ARG	2.5
1	A	1113	LYS	2.5
1	D	185	LEU	2.5
2	E	550	ASN	2.5
1	A	65	LEU	2.5
1	A	1218	LEU	2.5
1	A	134	PHE	2.5
1	D	104	LEU	2.5
1	D	189	ILE	2.5
2	H	485	ILE	2.5
1	C	111	ILE	2.5
1	A	1124	LYS	2.4
1	B	1165	ILE	2.4
1	A	1114	TYR	2.4
1	A	139	ASN	2.4
1	A	1129	LEU	2.4
1	C	105	VAL	2.4
2	G	543	SER	2.4
1	B	63	LYS	2.4
1	B	107	LEU	2.4
2	E	493	ARG	2.4
1	D	2	GLY	2.3
1	A	1148	TYR	2.3
1	A	1152	PRO	2.3
1	C	1145	ILE	2.3
2	F	486	VAL	2.3
1	D	99	GLN	2.3
1	B	1128	TYR	2.3
1	D	1122	ARG	2.3
1	D	117	THR	2.3
1	A	1142	LEU	2.3
1	B	32	ILE	2.3
1	B	69	GLY	2.3
1	B	182	TYR	2.2
1	A	107	LEU	2.2
1	A	1116	ALA	2.2
1	B	1120	LEU	2.2
2	F	528	PHE	2.2
1	A	1118	PRO	2.2
1	D	68	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	142	ILE	2.2
1	B	1063	LEU	2.1
1	B	185	LEU	2.1
1	D	187	GLU	2.1
1	A	1201	LEU	2.1
1	B	92	ALA	2.1
1	D	1107	PRO	2.1
1	B	1215	ILE	2.1
2	G	551	ILE	2.1
1	A	154	VAL	2.1
1	C	1128	TYR	2.1
1	B	1125	ASP	2.1
1	A	125	THR	2.0
1	D	1206	ARG	2.0
1	D	1059	LYS	2.0
1	D	1053	PHE	2.0
2	H	492	LEU	2.0
1	C	143	LYS	2.0
1	C	1149	GLN	2.0
1	D	1075	LEU	2.0
1	D	175	SER	2.0
1	A	128	TYR	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. 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	B-factors(Å^2)	Q<0.9
3	MG	C	2001	1/1	0.88	0.27	41,41,41,41	0

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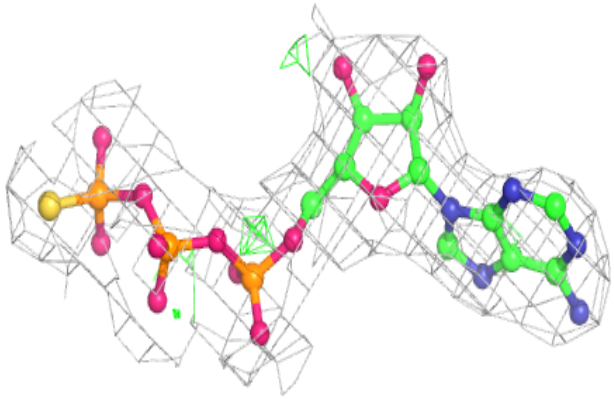
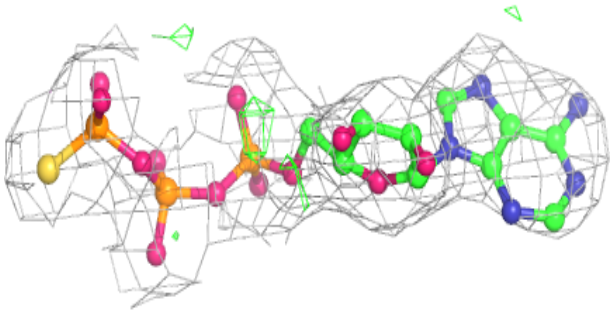
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	2001	1/1	0.89	0.17	37,37,37,37	0
3	MG	D	2001	1/1	0.91	0.24	35,35,35,35	0
3	MG	A	2001	1/1	0.96	0.21	38,38,38,38	0
4	AGS	B	2224	31/31	0.97	0.23	40,63,71,76	0
4	AGS	A	2224	31/31	0.98	0.23	42,50,58,60	0
4	AGS	C	2224	31/31	0.98	0.25	26,59,71,74	0
4	AGS	D	2224	31/31	0.98	0.24	24,55,60,63	0

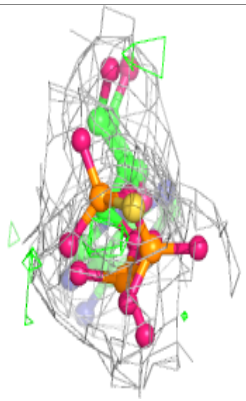
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AGS B 2224:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

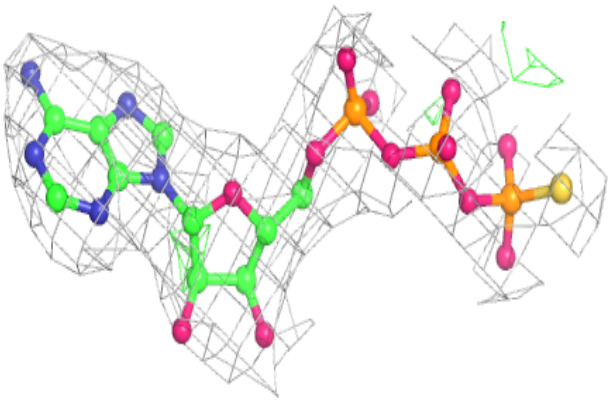


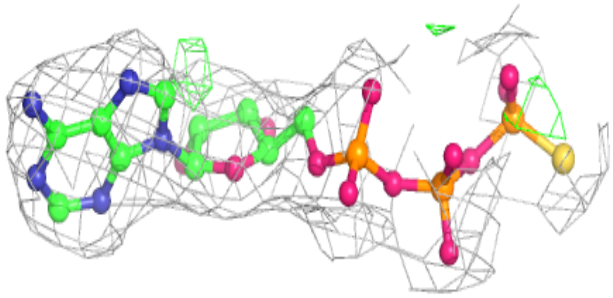


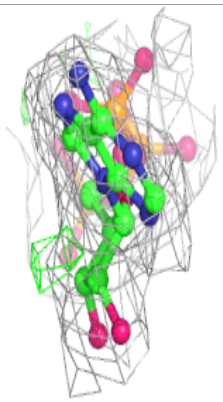


Electron density around AGS A 2224:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

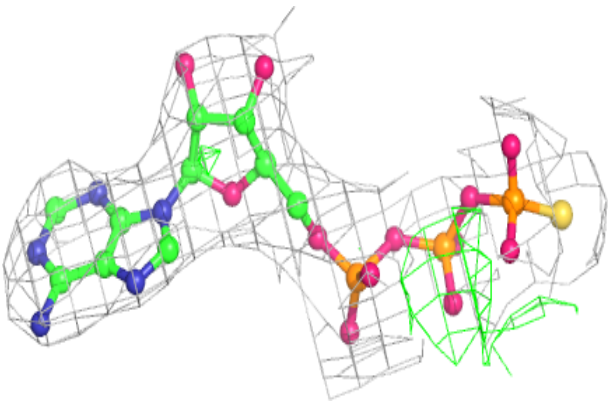


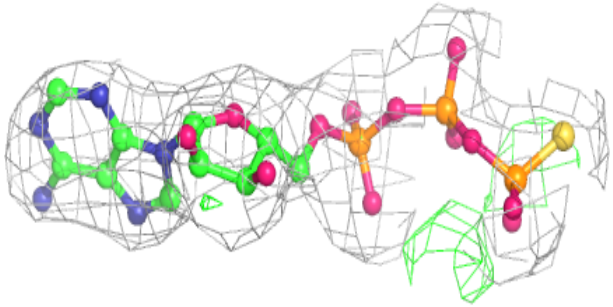


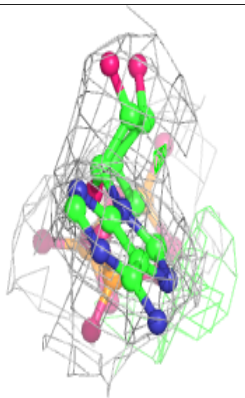


Electron density around AGS C 2224:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

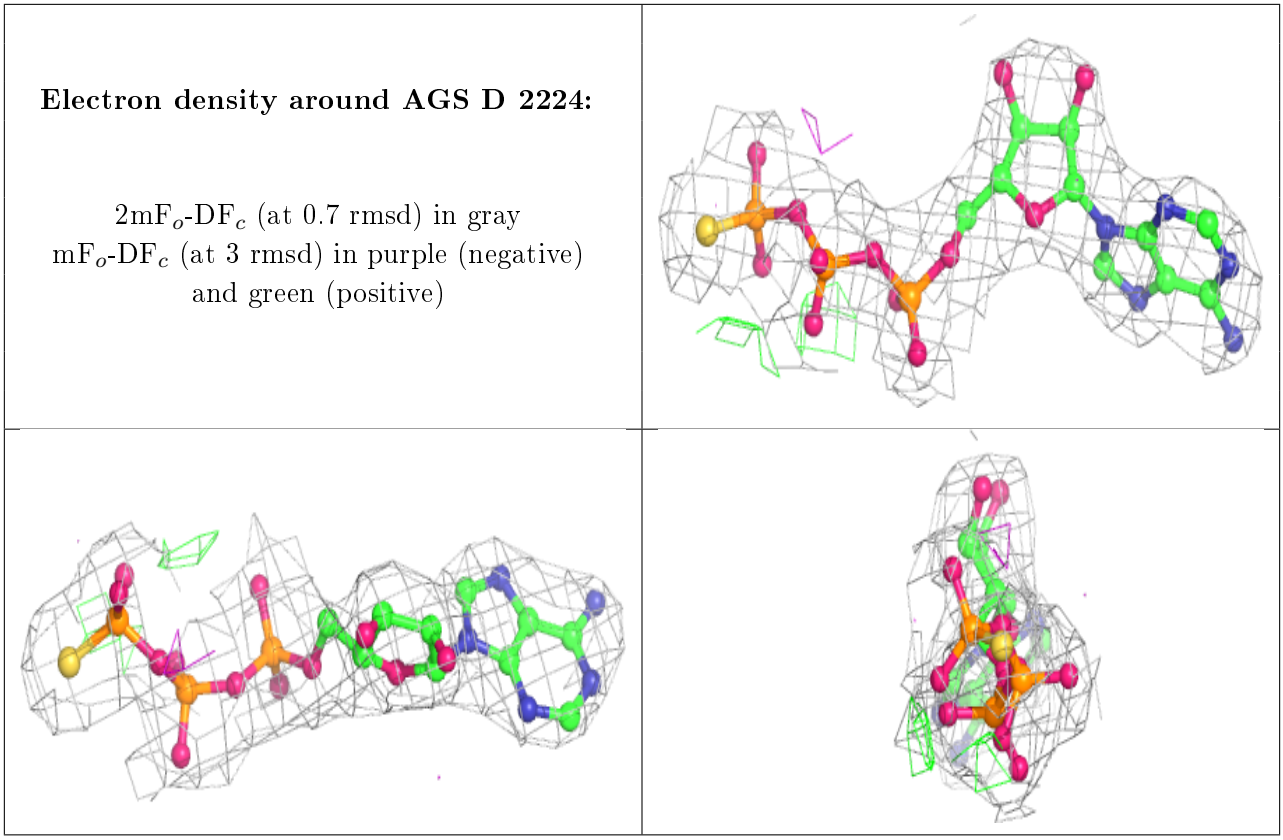






Electron density around AGS D 2224:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.