



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:16 PM GMT

PDB ID : 1SUS
Title : Crystal structure of alfalfa feruoyl coenzyme A 3-O-methyltransferase
Authors : Ferrer, J.-L.; Zubieta, C.; Dixon, R.A.; Noel, J.P.
Deposited on : 2004-03-26
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (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

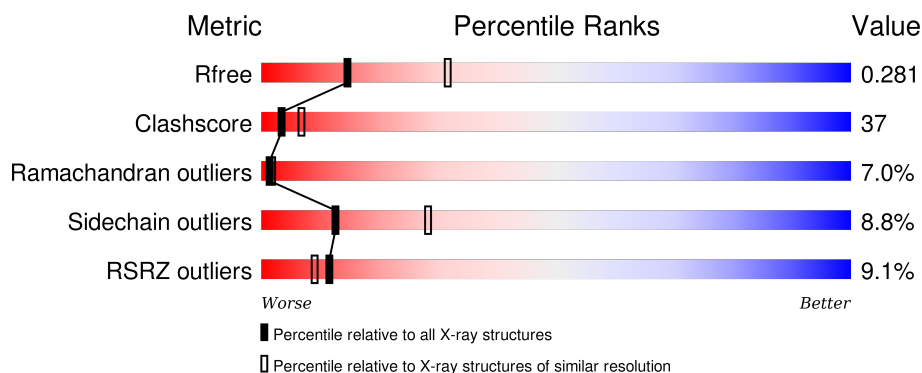
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	247	<div> <div>2%</div> <div>50%</div> <div>32%</div> <div>9%</div> <div>8%</div> </div>
1	B	247	<div> <div>5%</div> <div>59%</div> <div>27%</div> <div>5%</div> <div>8%</div> </div>
1	C	247	<div> <div>8%</div> <div>37%</div> <div>45%</div> <div>9%</div> <div>8%</div> </div>
1	D	247	<div> <div>18%</div> <div>28%</div> <div>53%</div> <div>10%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	B	306	-	-	-	X
3	SAH	B	302	-	-	-	X
3	SAH	C	303	-	-	-	X
4	SPF	A	401	X	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7447 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 Caffeoyle-CoA O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1807	1162	301	335	9			
1	B	227	Total	C	N	O	S	0	0	0
			1807	1162	301	335	9			
1	C	227	Total	C	N	O	S	0	0	0
			1807	1162	301	335	9			
1	D	227	Total	C	N	O	S	0	0	0
			1789	1150	295	335	9			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

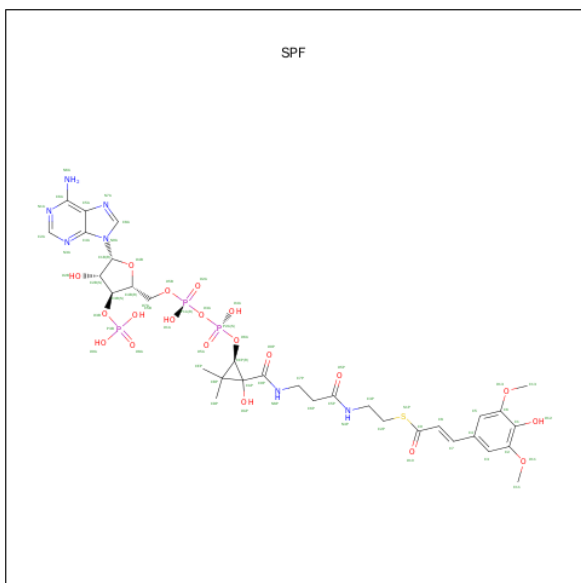
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 26	C 14	N 6	O 5	S 1	0	0
3	B	1	Total 26	C 14	N 6	O 5	S 1	0	0
3	C	1	Total 26	C 14	N 6	O 5	S 1	0	0
3	D	1	Total 26	C 14	N 6	O 5	S 1	0	0

- Molecule 4 is SINAPOYL COENZYME A (three-letter code: SPF) (formula: $\text{C}_{32}\text{H}_{44}\text{N}_7\text{O}_{20}\text{P}_3\text{S}$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			63	32	7	20	3	1		

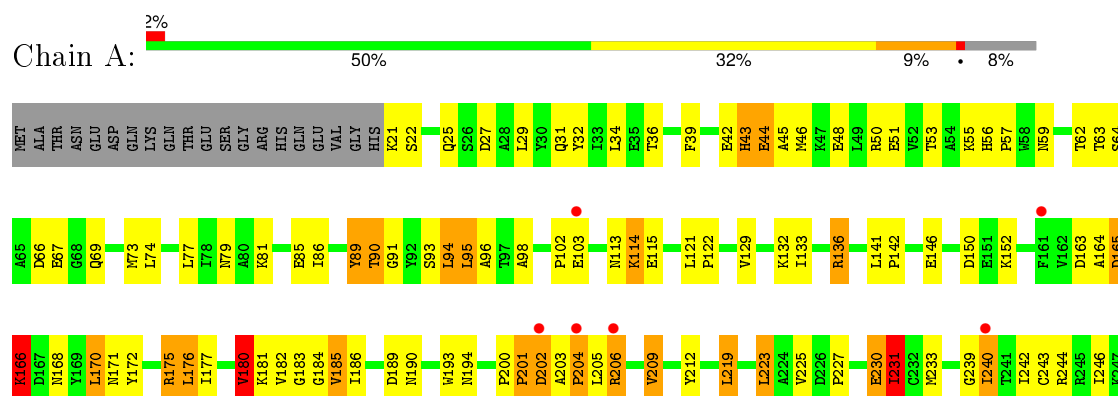
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	34	Total	O	0	0
			34	34		
5	C	11	Total	O	0	0
			11	11		
5	D	5	Total	O	0	0
			5	5		

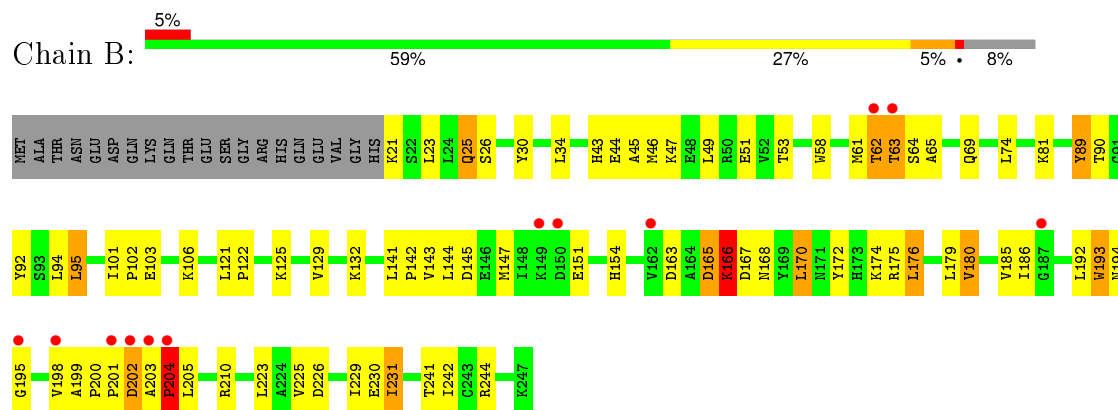
3 Residue-property plots

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.

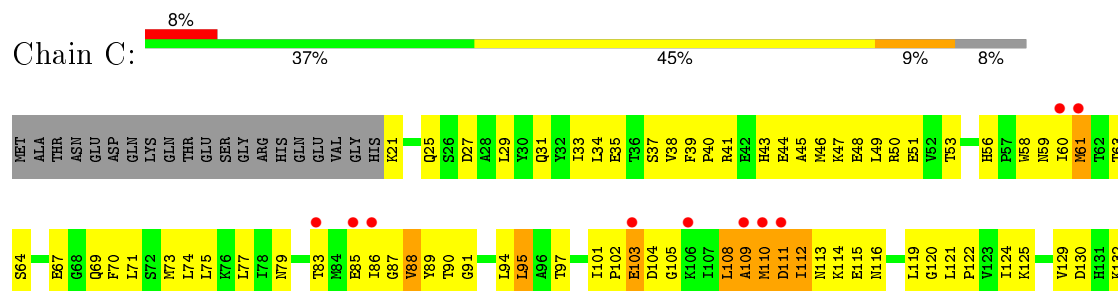
• Molecule 1: Caffeoyl-CoA O-methyltransferase

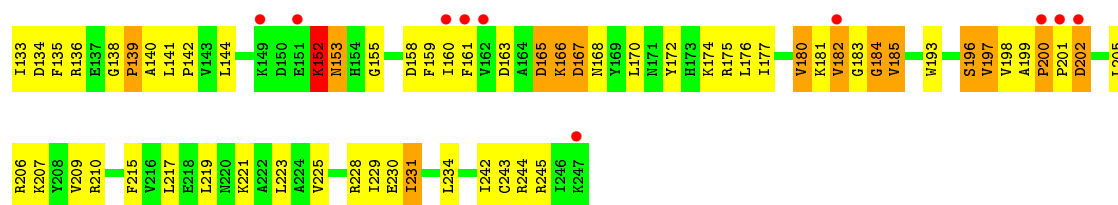


• Molecule 1: Caffeoyl-CoA O-methyltransferase

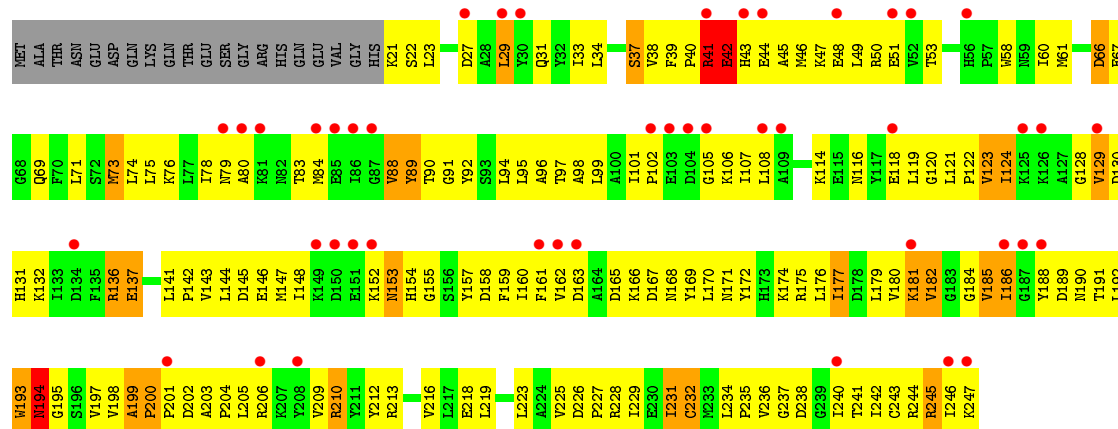


• Molecule 1: Caffeoyl-CoA O-methyltransferase





● Molecule 1: Caffeoyl-CoA O-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	60.85Å 136.49Å 332.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 25.08 – 2.72	Depositor EDS
% Data completeness (in resolution range)	93.7 (25.00-2.70) 93.9 (25.08-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.72Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.289 0.234 , 0.281	Depositor DCC
R_{free} test set	1789 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 35644 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7447	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SAH, SPF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/1844	0.72	2/2496 (0.1%)
1	B	0.46	0/1844	0.72	1/2496 (0.0%)
1	C	0.38	0/1844	0.63	0/2496
1	D	0.30	0/1824	0.53	0/2472
All	All	0.40	0/7356	0.66	3/9960 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	SER	N-CA-C	-5.29	96.71	111.00
1	A	184	GLY	N-CA-C	5.28	126.30	113.10
1	A	180	VAL	CB-CA-C	-5.25	101.43	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1807	0	1831	104	0
1	B	1807	0	1831	70	0
1	C	1807	0	1831	157	0
1	D	1789	0	1799	207	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	26	0	19	4	0
3	B	26	0	19	2	0
3	C	26	0	19	6	0
3	D	26	0	19	5	0
4	A	63	0	38	23	0
5	A	16	0	0	0	0
5	B	34	0	0	0	0
5	C	11	0	0	0	0
5	D	5	0	0	1	0
All	All	7447	0	7406	541	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 37.

All (541) 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)
4:A:401:SPF:C3P	4:A:401:SPF:C2P	1.77	1.62
1:D:141:LEU:HD21	1:D:175:ARG:HH21	1.15	1.07
1:B:165:ASP:O	1:B:166:LYS:HB2	1.57	1.03
1:A:165:ASP:O	1:A:166:LYS:HB2	1.59	0.98
1:C:141:LEU:H	1:C:141:LEU:HD12	1.33	0.92
1:A:193:TRP:CH2	4:A:401:SPF:H4	2.05	0.92
1:C:182:VAL:HG13	1:C:183:GLY:H	1.34	0.92
1:D:181:LYS:HA	1:D:245:ARG:HG3	1.54	0.90
1:D:185:VAL:HG13	1:D:186:ILE:H	1.37	0.89
1:C:185:VAL:HA	1:C:243:CYS:O	1.72	0.88
1:C:53:THR:OG1	1:C:90:THR:HG21	1.73	0.88
1:B:53:THR:HB	1:B:90:THR:HG21	1.56	0.88
1:C:61:MET:HE3	1:C:61:MET:H	1.38	0.86
1:D:141:LEU:HD21	1:D:175:ARG:NH2	1.90	0.86
1:A:193:TRP:HH2	4:A:401:SPF:H4	1.39	0.86
1:D:185:VAL:HG13	1:D:186:ILE:N	1.90	0.85
1:C:110:MET:HG3	1:C:111:ASP:OD1	1.76	0.85
1:C:181:LYS:HG3	1:C:182:VAL:H	1.39	0.84
1:A:113:ASN:O	1:A:114:LYS:HB3	1.75	0.84
1:A:53:THR:OG1	1:A:90:THR:HG21	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ILE:HG12	1:C:113:ASN:H	1.43	0.84
1:D:21:LYS:HG2	1:D:22:SER:H	1.42	0.82
1:D:124:ILE:HG22	1:D:130:ASP:HB3	1.62	0.82
1:D:146:GLU:HG3	1:D:147:MET:HG3	1.62	0.81
1:A:180:VAL:HG21	1:A:186:ILE:HD11	1.63	0.81
1:C:165:ASP:O	1:C:166:LYS:HB2	1.79	0.80
1:D:193:TRP:HE1	1:D:209:VAL:HA	1.46	0.80
4:A:401:SPF:N4P	4:A:401:SPF:C2P	2.45	0.80
1:C:198:VAL:HG12	1:C:199:ALA:H	1.45	0.79
1:D:152:LYS:HA	1:D:152:LYS:HE2	1.62	0.79
4:A:401:SPF:C3P	4:A:401:SPF:S1P	2.72	0.78
1:C:61:MET:N	1:C:61:MET:HE3	1.98	0.78
1:D:159:PHE:HA	1:D:185:VAL:HG11	1.64	0.78
1:D:231:ILE:HA	1:D:242:ILE:O	1.84	0.78
1:B:198:VAL:HG11	1:B:205:LEU:HD11	1.66	0.77
1:A:163:ASP:OD1	4:A:401:SPF:H133	1.85	0.77
1:B:89:TYR:O	1:B:90:THR:HB	1.84	0.77
1:C:205:LEU:HD21	1:C:210:ARG:NH2	1.99	0.77
1:D:34:LEU:HA	1:D:38:VAL:HG22	1.66	0.77
1:C:44:GLU:N	1:C:44:GLU:OE1	2.18	0.77
1:D:166:LYS:HB2	1:D:212:TYR:CD1	2.20	0.76
1:A:129:VAL:HG23	1:A:132:LYS:HE3	1.67	0.75
1:A:136:ARG:HG2	1:A:136:ARG:HH11	1.51	0.75
1:A:185:VAL:HA	1:A:243:CYS:O	1.87	0.75
1:A:85:GLU:OE2	1:A:93:SER:HB2	1.85	0.74
1:D:219:LEU:O	1:D:223:LEU:HB2	1.87	0.74
1:D:205:LEU:CD1	1:D:213:ARG:HH21	2.01	0.74
1:C:125:LYS:HD2	1:C:130:ASP:OD1	1.88	0.73
1:D:228:ARG:HH21	1:D:245:ARG:HH21	1.37	0.73
1:D:199:ALA:HB3	1:D:203:ALA:HB2	1.70	0.73
1:B:49:LEU:O	1:B:53:THR:HG22	1.88	0.72
1:A:67:GLU:OE2	1:A:240:ILE:HD12	1.89	0.72
1:A:42:GLU:OE2	1:A:50:ARG:NH2	2.22	0.72
1:D:205:LEU:HD13	1:D:213:ARG:HH21	1.53	0.71
1:D:184:GLY:O	1:D:185:VAL:HB	1.89	0.71
1:D:229:ILE:HA	1:D:244:ARG:O	1.90	0.71
1:B:230:GLU:O	1:B:231:ILE:HG12	1.91	0.70
1:C:45:ALA:HA	1:C:48:GLU:HB2	1.73	0.70
1:C:121:LEU:N	1:C:122:PRO:HD2	2.07	0.70
1:C:231:ILE:HA	1:C:242:ILE:O	1.91	0.70
1:D:47:LYS:O	1:D:51:GLU:HG3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:LEU:CD2	1:D:175:ARG:HH21	2.00	0.69
1:D:38:VAL:HG12	1:D:69:GLN:NE2	2.07	0.69
1:D:202:ASP:O	1:D:204:PRO:HD3	1.92	0.69
1:C:43:HIS:HB2	1:C:46:MET:HG2	1.74	0.68
1:C:60:ILE:HG23	1:C:61:MET:H	1.59	0.68
1:D:200:PRO:C	1:D:202:ASP:H	1.95	0.68
1:B:203:ALA:N	1:B:204:PRO:CD	2.57	0.68
1:C:110:MET:O	1:C:111:ASP:HB3	1.93	0.68
1:C:44:GLU:O	1:C:45:ALA:HB3	1.94	0.68
1:C:228:ARG:HH21	1:C:245:ARG:HH21	1.41	0.67
1:A:94:LEU:HD13	1:A:133:ILE:HD13	1.77	0.67
1:D:180:VAL:HG23	1:D:181:LYS:N	2.10	0.67
1:A:42:GLU:O	1:A:42:GLU:HG3	1.94	0.67
1:D:205:LEU:H	1:D:205:LEU:HD23	1.59	0.67
1:A:98:ALA:HB1	1:A:129:VAL:HG22	1.77	0.67
1:D:159:PHE:HD1	1:D:185:VAL:HG21	1.58	0.67
1:D:159:PHE:HD1	1:D:185:VAL:CG2	2.08	0.66
1:B:202:ASP:OD1	1:B:204:PRO:HB2	1.95	0.66
1:C:133:ILE:HD12	1:C:133:ILE:N	2.09	0.66
1:A:193:TRP:CH2	4:A:401:SPF:C3	2.78	0.66
1:A:44:GLU:HG3	1:A:45:ALA:N	2.09	0.66
1:B:230:GLU:HG3	1:B:244:ARG:CZ	2.25	0.66
1:A:212:TYR:CE2	4:A:401:SPF:H111	2.30	0.66
1:C:165:ASP:O	1:C:166:LYS:HE2	1.96	0.65
1:D:180:VAL:HG23	1:D:181:LYS:H	1.61	0.65
1:D:101:ILE:O	1:D:101:ILE:HD12	1.97	0.65
1:A:163:ASP:O	3:A:301:SAH:H5'1	1.96	0.65
1:C:120:GLY:C	1:C:122:PRO:HD2	2.17	0.65
1:D:160:ILE:O	1:D:186:ILE:HA	1.97	0.65
1:C:111:ASP:OD1	1:C:140:ALA:HB2	1.96	0.65
1:A:63:THR:HG23	3:A:301:SAH:OXT	1.96	0.65
1:C:43:HIS:HD2	1:C:46:MET:HG3	1.62	0.65
1:D:176:LEU:HA	1:D:179:LEU:HD23	1.79	0.64
1:D:38:VAL:HG12	1:D:69:GLN:HE21	1.61	0.64
1:B:180:VAL:HG21	1:B:186:ILE:HD11	1.78	0.64
1:C:87:GLY:HA2	3:C:303:SAH:H2	1.79	0.64
1:C:46:MET:HE1	1:C:95:LEU:HD13	1.80	0.64
1:B:230:GLU:HG3	1:B:244:ARG:NH2	2.13	0.64
1:D:170:LEU:HD12	1:D:218:GLU:HG2	1.79	0.64
1:A:43:HIS:O	1:A:44:GLU:HB3	1.97	0.64
1:C:182:VAL:HG13	1:C:183:GLY:N	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:TYR:HB3	3:B:302:SAH:HB2	1.80	0.64
1:D:83:THR:O	1:D:108:LEU:HD23	1.98	0.63
1:C:37:SER:O	1:C:69:GLN:NE2	2.31	0.63
1:C:198:VAL:HG12	1:C:199:ALA:N	2.14	0.62
1:C:108:LEU:O	1:C:110:MET:N	2.28	0.62
1:C:112:ILE:HG12	1:C:113:ASN:N	2.14	0.62
4:A:401:SPF:C5P	4:A:401:SPF:C2P	2.76	0.62
1:D:89:TYR:O	1:D:90:THR:HB	1.98	0.62
1:C:31:GLN:O	1:C:35:GLU:HG2	1.99	0.62
1:C:197:VAL:HG23	1:C:197:VAL:O	1.98	0.62
1:D:200:PRO:O	1:D:202:ASP:N	2.33	0.62
1:D:228:ARG:NH2	1:D:245:ARG:HH21	1.97	0.62
1:D:128:GLY:O	1:D:129:VAL:HG12	1.99	0.61
1:C:141:LEU:CD1	1:C:141:LEU:H	2.09	0.61
1:B:163:ASP:OD2	3:B:302:SAH:HG1	1.99	0.61
1:A:180:VAL:CG2	1:A:186:ILE:HD11	2.29	0.61
1:D:34:LEU:HA	1:D:38:VAL:CG2	2.30	0.61
1:B:170:LEU:HD12	1:B:174:LYS:HE2	1.81	0.61
1:C:217:LEU:O	1:C:221:LYS:HG2	2.00	0.61
1:D:34:LEU:HB3	1:D:39:PHE:CE1	2.36	0.61
1:B:200:PRO:N	1:B:201:PRO:HD2	2.16	0.61
1:C:86:ILE:HG12	1:C:110:MET:HG2	1.81	0.61
1:C:119:LEU:HD23	1:C:119:LEU:O	2.01	0.60
1:D:105:GLY:O	1:D:132:LYS:HD3	2.01	0.60
1:D:160:ILE:HD13	1:D:176:LEU:HD11	1.83	0.60
1:C:200:PRO:O	1:C:202:ASP:N	2.35	0.60
1:D:95:LEU:HD23	1:D:95:LEU:O	2.01	0.60
1:D:38:VAL:HG23	1:D:39:PHE:H	1.66	0.60
1:A:206:ARG:HE	1:A:206:ARG:N	1.99	0.60
1:A:163:ASP:OD1	4:A:401:SPF:C13	2.50	0.60
1:D:177:ILE:HD12	1:D:228:ARG:CZ	2.30	0.60
1:C:130:ASP:HA	1:C:133:ILE:HD13	1.84	0.60
1:B:205:LEU:HB2	1:B:210:ARG:NH1	2.17	0.60
1:D:146:GLU:HG3	1:D:147:MET:N	2.17	0.60
1:D:38:VAL:HG23	1:D:39:PHE:HD1	1.67	0.59
1:D:246:ILE:HG13	1:D:247:LYS:N	2.18	0.59
1:A:231:ILE:HA	1:A:242:ILE:O	2.02	0.59
1:A:171:ASN:O	1:A:175:ARG:HD3	2.03	0.59
1:D:46:MET:O	1:D:50:ARG:HG3	2.03	0.59
1:A:113:ASN:O	1:A:114:LYS:CB	2.47	0.59
1:D:106:LYS:HA	1:D:132:LYS:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ARG:HG2	1:A:136:ARG:NH1	2.17	0.59
1:C:43:HIS:CD2	1:C:46:MET:HG3	2.37	0.59
1:A:55:LYS:O	1:A:55:LYS:HD3	2.03	0.59
1:C:45:ALA:CA	1:C:48:GLU:HB2	2.33	0.58
4:A:401:SPF:C3P	4:A:401:SPF:O10	2.51	0.58
1:C:47:LYS:O	1:C:51:GLU:HG3	2.04	0.58
4:A:401:SPF:O12	4:A:401:SPF:H132	2.03	0.58
1:B:165:ASP:OD1	1:B:168:ASN:HB2	2.04	0.58
1:C:60:ILE:HG23	1:C:61:MET:HE3	1.85	0.58
1:A:201:PRO:O	1:A:202:ASP:HB3	2.02	0.58
1:C:103:GLU:HA	1:C:132:LYS:HE2	1.85	0.57
1:C:95:LEU:HG	1:C:124:ILE:HG12	1.85	0.57
1:A:21:LYS:HE2	4:A:401:SPF:OAP	2.04	0.57
1:C:103:GLU:HA	1:C:132:LYS:CE	2.33	0.57
1:D:177:ILE:HD13	1:D:177:ILE:O	2.05	0.57
1:D:212:TYR:O	1:D:216:VAL:HG23	2.04	0.57
1:D:184:GLY:HA2	1:D:245:ARG:HB2	1.86	0.57
1:D:165:ASP:C	1:D:166:LYS:HD2	2.25	0.57
1:C:141:LEU:HB2	1:C:142:PRO:HD3	1.87	0.57
1:D:38:VAL:HG23	1:D:39:PHE:N	2.20	0.57
1:A:46:MET:SD	1:A:95:LEU:HD13	2.45	0.56
1:C:228:ARG:NH2	1:C:245:ARG:HH21	2.03	0.56
1:D:114:LYS:HE3	1:D:137:GLU:HG2	1.87	0.56
1:D:141:LEU:HB3	1:D:142:PRO:HD3	1.87	0.56
1:D:21:LYS:HG2	1:D:22:SER:N	2.19	0.56
1:D:184:GLY:O	1:D:185:VAL:CB	2.53	0.56
1:D:185:VAL:CG1	1:D:186:ILE:N	2.62	0.56
1:A:21:LYS:N	4:A:401:SPF:O5P	2.39	0.56
1:C:103:GLU:HA	1:C:132:LYS:NZ	2.20	0.56
1:D:84:MET:HB3	1:D:160:ILE:HG12	1.88	0.56
1:C:67:GLU:O	1:C:71:LEU:HD22	2.06	0.56
1:B:203:ALA:O	1:B:205:LEU:N	2.31	0.55
1:A:74:LEU:O	1:A:74:LEU:HD12	2.07	0.55
1:D:27:ASP:O	1:D:31:GLN:HB2	2.06	0.55
1:D:71:LEU:O	1:D:75:LEU:HD13	2.06	0.55
1:B:203:ALA:N	1:B:204:PRO:HD2	2.21	0.55
1:A:193:TRP:HH2	4:A:401:SPF:C3	2.15	0.55
1:D:99:LEU:HD23	1:D:129:VAL:HG11	1.89	0.55
1:B:165:ASP:O	1:B:166:LYS:CB	2.43	0.55
1:D:182:VAL:H	1:D:245:ARG:HH11	1.53	0.55
1:B:226:ASP:HB3	1:B:229:ILE:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:VAL:O	1:C:89:TYR:HB3	2.06	0.55
1:D:200:PRO:C	1:D:202:ASP:N	2.60	0.55
4:A:401:SPF:O12	4:A:401:SPF:C11	2.55	0.55
4:A:401:SPF:O10	4:A:401:SPF:H32	2.07	0.55
1:D:234:LEU:HB3	1:D:236:VAL:HG23	1.89	0.55
1:C:183:GLY:O	1:C:185:VAL:N	2.40	0.54
1:D:158:ASP:O	1:D:185:VAL:HG11	2.07	0.54
1:C:163:ASP:OD2	3:C:303:SAH:HA	2.07	0.54
1:D:39:PHE:HB2	1:D:40:PRO:HD3	1.89	0.54
1:B:34:LEU:HD22	1:B:65:ALA:HB3	1.89	0.54
1:C:89:TYR:O	1:C:90:THR:HB	2.08	0.54
1:D:83:THR:CG2	1:D:159:PHE:HB3	2.38	0.54
1:D:48:GLU:OE1	1:D:123:VAL:HG13	2.08	0.54
1:C:206:ARG:O	1:C:209:VAL:HG22	2.07	0.54
1:D:160:ILE:HD12	1:D:180:VAL:HG13	1.89	0.54
1:A:43:HIS:O	1:A:44:GLU:CB	2.55	0.54
1:C:70:PHE:CZ	1:C:234:LEU:HD12	2.43	0.54
1:D:162:VAL:HG12	1:D:169:TYR:HE1	1.71	0.54
1:D:184:GLY:CA	1:D:245:ARG:H	2.21	0.54
1:B:165:ASP:HB2	1:B:167:ASP:OD1	2.08	0.53
1:A:172:TYR:HB3	1:A:176:LEU:HD22	1.89	0.53
1:A:182:VAL:O	1:A:183:GLY:C	2.47	0.53
1:C:205:LEU:H	1:C:205:LEU:HD23	1.73	0.53
1:A:142:PRO:O	1:A:146:GLU:HG3	2.09	0.53
1:D:189:ASP:O	1:D:190:ASN:HB2	2.08	0.53
1:C:56:HIS:HE1	1:C:58:TRP:HB2	1.73	0.53
1:A:165:ASP:O	1:A:166:LYS:HE2	2.08	0.53
1:D:181:LYS:HB3	1:D:245:ARG:HH12	1.73	0.53
1:D:166:LYS:HA	1:D:169:TYR:CD2	2.43	0.53
1:A:32:TYR:O	1:A:36:THR:HG23	2.09	0.53
1:C:166:LYS:HE3	1:C:193:TRP:CZ3	2.44	0.53
1:A:59:ASN:O	1:A:62:THR:HG22	2.09	0.53
1:B:199:ALA:O	1:B:202:ASP:HB3	2.09	0.53
1:C:49:LEU:HD22	1:C:95:LEU:HD12	1.90	0.53
1:C:73:MET:HE3	1:C:77:LEU:HG	1.91	0.52
1:D:206:ARG:HB2	1:D:209:VAL:HG12	1.90	0.52
1:C:46:MET:CE	1:C:95:LEU:HD13	2.38	0.52
1:A:230:GLU:OE1	1:A:246:ILE:HG21	2.09	0.52
1:D:73:MET:HA	1:D:73:MET:CE	2.39	0.52
1:C:141:LEU:HD12	1:C:141:LEU:N	2.14	0.52
1:C:121:LEU:N	1:C:122:PRO:CD	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:ASP:HB3	3:D:304:SAH:N7	2.25	0.52
1:D:29:LEU:O	1:D:33:ILE:HG13	2.09	0.52
1:A:150:ASP:OD1	1:A:152:LYS:HB2	2.09	0.52
1:D:53:THR:HG22	1:D:53:THR:O	2.09	0.52
1:A:193:TRP:CZ3	4:A:401:SPF:C3	2.93	0.52
1:D:83:THR:HG22	1:D:159:PHE:HB3	1.91	0.52
1:D:128:GLY:C	1:D:130:ASP:H	2.14	0.52
1:D:74:LEU:O	1:D:78:ILE:HG12	2.10	0.52
1:D:42:GLU:OE2	1:D:47:LYS:HE3	2.09	0.51
1:D:21:LYS:HE3	1:D:22:SER:O	2.10	0.51
1:C:39:PHE:HB2	1:C:40:PRO:HD3	1.92	0.51
1:D:98:ALA:HB1	1:D:129:VAL:HG13	1.92	0.51
1:C:46:MET:O	1:C:50:ARG:HB2	2.10	0.51
1:A:244:ARG:HD3	1:C:73:MET:HE1	1.93	0.51
1:B:121:LEU:N	1:B:122:PRO:HD2	2.25	0.51
1:A:180:VAL:HG21	1:A:186:ILE:CD1	2.37	0.51
1:A:239:GLY:C	1:A:240:ILE:HD13	2.31	0.51
1:C:56:HIS:CE1	1:C:58:TRP:HB2	2.46	0.51
1:C:110:MET:O	1:C:136:ARG:HB2	2.11	0.51
1:C:85:GLU:O	1:C:110:MET:HB3	2.11	0.51
1:C:34:LEU:HD23	1:C:38:VAL:HG21	1.93	0.51
1:B:223:LEU:HD23	1:B:241:THR:HG21	1.93	0.51
1:A:32:TYR:CE1	1:A:36:THR:HG21	2.46	0.51
1:C:184:GLY:O	1:C:185:VAL:HB	2.09	0.50
1:C:46:MET:CE	1:C:95:LEU:HD22	2.40	0.50
1:A:231:ILE:O	1:A:231:ILE:HG13	2.10	0.50
1:C:64:SER:HB2	1:C:67:GLU:HG3	1.92	0.50
1:D:170:LEU:HD23	1:D:170:LEU:O	2.11	0.50
1:B:25:GLN:O	1:B:26:SER:HB3	2.11	0.50
1:B:205:LEU:HB2	1:B:210:ARG:HH12	1.76	0.50
1:D:188:TYR:CD1	1:D:223:LEU:HD21	2.46	0.50
1:B:121:LEU:HG	1:B:125:LYS:HE3	1.92	0.50
1:B:225:VAL:O	1:B:225:VAL:HG12	2.11	0.50
1:D:95:LEU:HD23	1:D:99:LEU:HG	1.94	0.50
1:D:162:VAL:HG12	1:D:169:TYR:CE1	2.46	0.50
1:D:159:PHE:CD1	1:D:185:VAL:HG21	2.44	0.50
1:D:185:VAL:HG22	1:D:186:ILE:N	2.27	0.50
1:C:196:SER:O	1:C:198:VAL:HG23	2.11	0.50
1:D:191:THR:HG21	1:D:241:THR:OG1	2.11	0.49
1:C:89:TYR:HA	1:C:116:ASN:HB2	1.93	0.49
1:A:98:ALA:HB1	1:A:129:VAL:CG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:TYR:HB3	1:B:176:LEU:HD22	1.94	0.49
1:B:231:ILE:HA	1:B:242:ILE:O	2.13	0.49
1:D:118:GLU:O	1:D:122:PRO:HD3	2.12	0.49
1:A:206:ARG:HB2	1:A:209:VAL:HG13	1.94	0.49
1:B:46:MET:HE3	1:B:92:TYR:CE1	2.47	0.49
3:A:301:SAH:HG2	4:A:401:SPF:H131	1.94	0.49
1:D:234:LEU:O	1:D:236:VAL:N	2.37	0.49
1:D:193:TRP:NE1	1:D:209:VAL:HA	2.21	0.49
1:D:166:LYS:N	1:D:166:LYS:HD2	2.27	0.49
1:C:49:LEU:CD2	1:C:95:LEU:HD12	2.43	0.49
1:D:200:PRO:HB2	1:D:202:ASP:OD2	2.12	0.49
1:D:122:PRO:C	1:D:124:ILE:H	2.15	0.49
1:D:95:LEU:O	1:D:99:LEU:HG	2.13	0.49
1:B:180:VAL:CG2	1:B:186:ILE:HD11	2.41	0.49
1:D:144:LEU:HD11	1:D:176:LEU:HD13	1.95	0.49
1:D:229:ILE:HD12	1:D:243:CYS:SG	2.53	0.49
1:D:176:LEU:CA	1:D:179:LEU:HD23	2.42	0.48
1:D:180:VAL:O	1:D:181:LYS:O	2.31	0.48
1:C:133:ILE:CD1	1:C:133:ILE:N	2.75	0.48
1:B:106:LYS:HE2	1:B:106:LYS:HA	1.95	0.48
1:C:43:HIS:HB3	1:C:44:GLU:OE1	2.12	0.48
1:D:108:LEU:HG	1:D:157:TYR:OH	2.13	0.48
1:D:185:VAL:HG22	1:D:186:ILE:H	1.77	0.48
1:D:166:LYS:HA	1:D:169:TYR:CE2	2.49	0.48
1:A:176:LEU:O	1:A:180:VAL:HG23	2.13	0.48
1:D:184:GLY:HA2	1:D:245:ARG:H	1.79	0.48
1:D:22:SER:OG	1:D:23:LEU:N	2.46	0.48
1:D:121:LEU:N	1:D:122:PRO:CD	2.76	0.48
1:D:219:LEU:C	1:D:219:LEU:HD13	2.33	0.48
1:B:62:THR:HG23	1:B:63:THR:N	2.28	0.48
1:B:151:GLU:HA	1:B:154:HIS:CD2	2.48	0.48
1:A:170:LEU:CD2	1:A:219:LEU:HA	2.43	0.48
1:A:240:ILE:HD13	1:A:240:ILE:N	2.29	0.48
1:D:116:ASN:O	1:D:119:LEU:HB3	2.13	0.48
1:D:84:MET:HB2	1:D:157:TYR:CE2	2.49	0.48
1:A:231:ILE:HG12	1:C:41:ARG:HD3	1.96	0.48
1:D:192:LEU:O	1:D:193:TRP:C	2.52	0.48
1:A:230:GLU:O	1:A:231:ILE:HG12	2.14	0.48
1:A:200:PRO:HG2	1:A:203:ALA:HB2	1.96	0.48
1:B:30:TYR:CE1	1:B:34:LEU:HD11	2.49	0.48
1:C:152:LYS:HA	1:C:152:LYS:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:LEU:HD21	1:D:97:THR:HG23	1.96	0.48
1:A:244:ARG:HB2	1:C:73:MET:CE	2.44	0.47
1:D:226:ASP:HB3	1:D:229:ILE:HG12	1.96	0.47
1:D:165:ASP:OD2	3:D:304:SAH:N6	2.47	0.47
1:C:196:SER:OG	1:C:197:VAL:N	2.45	0.47
1:B:230:GLU:OE2	1:B:244:ARG:NH2	2.46	0.47
1:D:41:ARG:HA	1:D:41:ARG:CZ	2.44	0.47
1:D:41:ARG:HG3	1:D:41:ARG:HH11	1.79	0.47
1:C:115:GLU:OE1	1:C:115:GLU:HA	2.14	0.47
1:A:25:GLN:NE2	1:C:21:LYS:NZ	2.62	0.47
1:C:158:ASP:O	1:C:184:GLY:O	2.33	0.47
1:C:229:ILE:HA	1:C:244:ARG:O	2.15	0.47
1:A:233:MET:CE	1:C:37:SER:HB2	2.44	0.47
1:D:160:ILE:HB	1:D:186:ILE:HG12	1.97	0.47
1:C:85:GLU:OE2	1:C:94:LEU:HB2	2.15	0.47
1:A:53:THR:OG1	1:A:90:THR:CG2	2.56	0.47
1:C:182:VAL:HG22	1:C:183:GLY:N	2.28	0.47
1:D:225:VAL:O	1:D:227:PRO:HD3	2.15	0.47
1:B:143:VAL:HG12	1:B:147:MET:HE2	1.97	0.47
1:C:181:LYS:CG	1:C:182:VAL:H	2.16	0.47
1:C:111:ASP:OD2	1:C:138:GLY:O	2.33	0.47
1:D:209:VAL:HG13	1:D:210:ARG:N	2.29	0.47
1:D:89:TYR:C	1:D:91:GLY:H	2.18	0.47
1:C:133:ILE:H	1:C:133:ILE:HD12	1.78	0.46
1:D:163:ASP:OD2	3:D:304:SAH:HB1	2.16	0.46
1:D:159:PHE:HA	1:D:185:VAL:CG1	2.41	0.46
1:D:180:VAL:CG2	1:D:181:LYS:N	2.78	0.46
1:D:114:LYS:HE3	1:D:137:GLU:CG	2.44	0.46
1:C:88:VAL:HG13	1:C:91:GLY:HA2	1.96	0.46
1:C:109:ALA:O	1:C:110:MET:C	2.53	0.46
1:C:112:ILE:HG13	3:C:303:SAH:N3	2.29	0.46
1:C:176:LEU:O	1:C:180:VAL:HG22	2.14	0.46
1:C:167:ASP:HB3	1:C:215:PHE:CE1	2.50	0.46
1:D:107:ILE:C	1:D:108:LEU:HD22	2.36	0.46
1:D:179:LEU:HD22	1:D:179:LEU:N	2.30	0.46
1:C:60:ILE:CG2	1:C:61:MET:HE3	2.45	0.46
1:A:185:VAL:H	1:A:244:ARG:HA	1.79	0.46
1:D:129:VAL:HA	1:D:131:HIS:CE1	2.51	0.46
1:C:230:GLU:O	1:C:231:ILE:HG12	2.15	0.46
1:B:47:LYS:O	1:B:51:GLU:HG3	2.16	0.46
1:A:163:ASP:OD2	3:A:301:SAH:HB1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:VAL:CG2	1:D:181:LYS:H	2.28	0.46
1:D:185:VAL:CG1	1:D:186:ILE:H	2.09	0.46
1:A:177:ILE:O	1:A:177:ILE:HG13	2.16	0.46
1:B:172:TYR:HB3	1:B:176:LEU:CD2	2.45	0.46
1:A:46:MET:HE1	1:A:96:ALA:HB2	1.97	0.46
1:B:45:ALA:HB1	1:B:95:LEU:HD11	1.98	0.46
1:A:56:HIS:ND1	1:A:57:PRO:HD2	2.30	0.46
1:D:181:LYS:HB3	1:D:245:ARG:NH1	2.30	0.46
1:B:200:PRO:CD	1:B:201:PRO:HD2	2.45	0.46
1:C:44:GLU:O	1:C:44:GLU:HG2	2.16	0.46
1:D:232:CYS:HB3	1:D:242:ILE:HG13	1.98	0.46
1:C:88:VAL:HG12	1:C:89:TYR:N	2.31	0.46
1:B:176:LEU:O	1:B:180:VAL:HG22	2.15	0.46
1:A:200:PRO:HA	1:A:201:PRO:HD3	1.80	0.46
1:D:136:ARG:HH11	1:D:136:ARG:HG2	1.81	0.46
1:A:225:VAL:HG12	1:A:225:VAL:O	2.15	0.46
1:B:43:HIS:CD2	1:B:45:ALA:H	2.35	0.45
1:D:120:GLY:O	1:D:124:ILE:HG13	2.16	0.45
1:D:131:HIS:CD2	1:D:132:LYS:HZ3	2.34	0.45
1:D:161:PHE:CE1	1:D:189:ASP:HB2	2.51	0.45
1:A:27:ASP:O	1:A:31:GLN:HG2	2.16	0.45
1:D:80:ALA:HB1	1:D:83:THR:CG2	2.47	0.45
1:C:29:LEU:O	1:C:33:ILE:HG13	2.16	0.45
1:D:185:VAL:O	1:D:243:CYS:O	2.33	0.45
1:D:114:LYS:O	1:D:118:GLU:HG3	2.17	0.45
1:D:143:VAL:O	1:D:146:GLU:HG2	2.15	0.45
1:D:123:VAL:O	1:D:123:VAL:HG12	2.16	0.45
1:B:46:MET:SD	1:B:95:LEU:HD13	2.56	0.45
1:B:165:ASP:OD1	1:B:166:LYS:N	2.48	0.45
1:D:144:LEU:O	1:D:148:ILE:HG12	2.17	0.45
1:A:165:ASP:HB2	1:A:168:ASN:HB2	1.98	0.45
1:D:229:ILE:HB	1:D:243:CYS:HB3	1.99	0.45
1:A:225:VAL:O	1:A:227:PRO:HD3	2.17	0.45
1:C:101:ILE:HB	1:C:102:PRO:HD2	1.99	0.45
1:C:133:ILE:HG22	1:C:134:ASP:N	2.31	0.45
1:D:101:ILE:HA	5:D:310:HOH:O	2.16	0.45
1:D:205:LEU:HD12	1:D:209:VAL:HG22	1.99	0.45
1:A:202:ASP:C	1:A:204:PRO:HD3	2.37	0.45
1:A:89:TYR:O	1:A:91:GLY:N	2.41	0.45
1:D:160:ILE:HD13	1:D:176:LEU:CD1	2.47	0.45
1:C:230:GLU:OE1	1:C:244:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:THR:CG2	1:D:90:THR:HG21	2.46	0.45
1:A:225:VAL:CG1	1:A:225:VAL:O	2.64	0.45
1:A:189:ASP:O	1:A:190:ASN:HB2	2.16	0.45
1:A:166:LYS:C	1:A:168:ASN:H	2.20	0.45
1:D:198:VAL:HG22	1:D:199:ALA:N	2.32	0.45
1:C:205:LEU:HD21	1:C:210:ARG:HH21	1.79	0.44
1:D:165:ASP:OD1	1:D:168:ASN:HB2	2.17	0.44
1:B:176:LEU:O	1:B:180:VAL:CG2	2.65	0.44
1:C:114:LYS:HG3	1:C:115:GLU:H	1.82	0.44
1:C:144:LEU:HD23	1:C:175:ARG:HB2	1.98	0.44
1:D:108:LEU:N	1:D:108:LEU:HD22	2.33	0.44
1:D:38:VAL:HG11	1:D:66:ASP:HA	1.99	0.44
1:B:81:LYS:HG2	1:B:102:PRO:CG	2.47	0.44
1:D:145:ASP:OD1	1:D:175:ARG:HD2	2.17	0.44
1:C:109:ALA:CB	1:C:133:ILE:HG23	2.47	0.44
1:A:129:VAL:HG23	1:A:132:LYS:CE	2.44	0.44
1:A:22:SER:O	1:C:25:GLN:NE2	2.46	0.44
1:D:181:LYS:CB	1:D:245:ARG:NH1	2.81	0.44
1:C:209:VAL:HG23	1:C:210:ARG:N	2.32	0.44
1:B:193:TRP:O	1:B:195:GLY:N	2.45	0.44
1:D:60:ILE:HG13	1:D:60:ILE:O	2.17	0.44
1:A:165:ASP:CB	1:A:168:ASN:HB2	2.48	0.44
1:D:58:TRP:HB3	1:D:61:MET:CE	2.48	0.44
1:C:44:GLU:CD	1:C:44:GLU:H	2.19	0.44
1:A:244:ARG:HB2	1:C:73:MET:HE1	2.00	0.44
1:C:67:GLU:O	1:C:71:LEU:CD2	2.65	0.44
1:B:143:VAL:HG12	1:B:147:MET:CE	2.48	0.44
1:D:154:HIS:HB3	1:D:181:LYS:HE2	1.99	0.43
1:D:172:TYR:O	1:D:176:LEU:HB2	2.18	0.43
1:C:61:MET:CE	1:C:61:MET:H	2.21	0.43
1:D:190:ASN:HD22	1:D:190:ASN:N	2.13	0.43
1:C:198:VAL:CG1	1:C:199:ALA:H	2.25	0.43
1:B:101:ILE:HB	1:B:102:PRO:HD2	2.00	0.43
1:D:194:ASN:HB3	1:D:195:GLY:H	1.65	0.43
1:D:192:LEU:HB2	1:D:238:ASP:O	2.18	0.43
1:C:133:ILE:H	1:C:133:ILE:CD1	2.32	0.43
1:D:101:ILE:C	1:D:101:ILE:HD12	2.39	0.43
1:B:43:HIS:HD2	1:B:45:ALA:H	1.67	0.43
4:A:401:SPF:O12	4:A:401:SPF:H113	2.18	0.43
1:C:182:VAL:O	1:C:245:ARG:O	2.37	0.43
1:A:103:GLU:HA	1:A:103:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:GLY:C	1:D:157:TYR:H	2.22	0.43
1:D:128:GLY:C	1:D:130:ASP:N	2.72	0.43
1:C:125:LYS:HD2	1:C:130:ASP:CG	2.39	0.43
1:D:45:ALA:HB1	1:D:95:LEU:HD11	2.01	0.43
1:D:189:ASP:OD2	1:D:190:ASN:ND2	2.52	0.43
1:A:42:GLU:O	1:A:42:GLU:CG	2.65	0.43
1:A:170:LEU:HD22	1:A:219:LEU:HD23	2.00	0.43
1:D:234:LEU:C	1:D:236:VAL:H	2.19	0.43
1:C:111:ASP:CB	1:C:136:ARG:O	2.67	0.43
1:C:86:ILE:HG12	1:C:110:MET:CG	2.46	0.43
1:C:228:ARG:NH2	1:C:245:ARG:NH2	2.67	0.43
1:C:109:ALA:HB2	1:C:133:ILE:HG23	2.00	0.43
1:D:49:LEU:HD23	1:D:92:TYR:HA	2.00	0.43
1:B:192:LEU:HA	1:B:192:LEU:HD23	1.88	0.43
1:A:48:GLU:O	1:A:51:GLU:HB2	2.19	0.43
1:C:112:ILE:HA	3:C:303:SAH:C2	2.48	0.42
1:A:56:HIS:CG	1:A:57:PRO:HD2	2.54	0.42
1:D:141:LEU:HD23	1:D:141:LEU:O	2.18	0.42
1:A:163:ASP:O	4:A:401:SPF:H131	2.19	0.42
1:A:73:MET:O	1:A:77:LEU:HG	2.19	0.42
1:C:112:ILE:HG22	1:C:135:PHE:CZ	2.55	0.42
1:C:46:MET:HE1	1:C:95:LEU:HB3	2.00	0.42
1:A:86:ILE:HG22	1:A:164:ALA:HB2	2.01	0.42
1:D:231:ILE:HG22	1:D:243:CYS:SG	2.59	0.42
1:C:153:ASN:HA	1:C:153:ASN:HD22	1.55	0.42
1:C:75:LEU:CD1	1:C:97:THR:HG23	2.50	0.42
1:C:163:ASP:OD1	3:C:303:SAH:HG1	2.18	0.42
1:D:166:LYS:HE3	1:D:193:TRP:CZ3	2.54	0.42
1:B:201:PRO:O	1:B:203:ALA:N	2.53	0.42
1:A:200:PRO:O	1:A:202:ASP:N	2.53	0.42
1:D:67:GLU:OE2	1:D:240:ILE:HG13	2.18	0.42
1:C:182:VAL:O	1:C:245:ARG:HB3	2.20	0.42
1:C:103:GLU:HA	1:C:132:LYS:HZ1	1.83	0.42
1:C:160:ILE:HD12	1:C:180:VAL:HG13	2.01	0.42
1:C:160:ILE:CD1	1:C:180:VAL:HG13	2.49	0.42
1:D:197:VAL:O	1:D:197:VAL:HG22	2.19	0.42
1:A:194:ASN:OD1	4:A:401:SPF:H22	2.20	0.42
1:D:165:ASP:OD1	1:D:165:ASP:C	2.58	0.42
1:B:200:PRO:HD2	1:B:201:PRO:HD2	2.00	0.42
1:B:61:MET:HB2	1:B:62:THR:H	1.57	0.42
1:B:89:TYR:O	1:B:90:THR:CB	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:GLY:O	1:D:130:ASP:N	2.53	0.42
1:C:209:VAL:CG2	1:C:210:ARG:N	2.83	0.42
1:A:121:LEU:N	1:A:122:PRO:CD	2.83	0.42
1:D:184:GLY:HA3	1:D:245:ARG:H	1.83	0.41
1:D:232:CYS:SG	1:D:234:LEU:HD21	2.60	0.41
1:C:43:HIS:HB2	1:C:46:MET:CG	2.47	0.41
1:B:21:LYS:O	1:B:21:LYS:HG2	2.21	0.41
1:D:159:PHE:HA	1:D:185:VAL:HG21	2.01	0.41
1:C:165:ASP:HB2	1:C:168:ASN:HD22	1.85	0.41
1:D:163:ASP:OD1	1:D:189:ASP:HB3	2.20	0.41
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.84	0.41
1:D:46:MET:CE	1:D:96:ALA:HB2	2.50	0.41
1:A:201:PRO:O	1:A:202:ASP:CB	2.68	0.41
1:C:207:LYS:HB3	1:C:207:LYS:HE3	1.93	0.41
1:D:43:HIS:O	1:D:44:GLU:HB3	2.20	0.41
1:A:166:LYS:HE2	4:A:401:SPF:H112	2.01	0.41
1:D:61:MET:SD	3:D:304:SAH:SD	3.19	0.41
1:A:175:ARG:N	1:A:175:ARG:CD	2.84	0.41
1:B:89:TYR:CD2	1:B:89:TYR:O	2.73	0.41
1:C:108:LEU:C	1:C:110:MET:N	2.74	0.41
1:C:58:TRP:O	1:C:59:ASN:C	2.58	0.41
1:C:219:LEU:C	1:C:219:LEU:HD13	2.41	0.41
1:C:159:PHE:CZ	1:C:161:PHE:HB2	2.54	0.41
1:C:155:GLY:HA3	1:C:181:LYS:HD2	2.03	0.41
1:D:177:ILE:HD13	1:D:177:ILE:C	2.41	0.41
1:B:81:LYS:HG2	1:B:102:PRO:HG3	2.02	0.41
1:A:81:LYS:HG3	1:A:102:PRO:CG	2.51	0.41
1:C:114:LYS:HG3	1:C:115:GLU:N	2.36	0.41
1:C:60:ILE:HG23	1:C:61:MET:N	2.31	0.41
1:C:165:ASP:O	1:C:166:LYS:CB	2.56	0.41
1:D:88:VAL:O	3:D:304:SAH:HA	2.21	0.41
1:B:145:ASP:OD1	1:B:175:ARG:NE	2.53	0.41
1:D:171:ASN:O	1:D:172:TYR:C	2.58	0.41
1:D:23:LEU:HD12	1:D:237:GLY:O	2.21	0.41
1:D:205:LEU:CD1	1:D:213:ARG:NH2	2.79	0.41
1:C:38:VAL:O	1:C:39:PHE:C	2.58	0.41
1:C:114:LYS:O	1:C:115:GLU:OE1	2.39	0.41
1:B:193:TRP:HA	1:B:193:TRP:CE3	2.56	0.41
1:C:75:LEU:HD11	1:C:97:THR:HG23	2.02	0.41
1:B:141:LEU:HB3	1:B:142:PRO:HD3	2.01	0.41
1:C:63:THR:O	1:C:63:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:HB3	1:A:39:PHE:CE2	2.55	0.41
1:D:95:LEU:C	1:D:95:LEU:HD23	2.40	0.41
1:D:89:TYR:O	1:D:90:THR:CB	2.68	0.41
1:B:129:VAL:O	1:B:132:LYS:HG3	2.21	0.41
1:B:23:LEU:HD21	1:B:194:ASN:HA	2.03	0.41
1:D:180:VAL:CG2	1:D:186:ILE:HD11	2.51	0.40
1:D:180:VAL:HG21	1:D:186:ILE:HD11	2.03	0.40
1:A:181:LYS:HE3	1:A:181:LYS:HB3	1.78	0.40
1:D:84:MET:O	1:D:160:ILE:HA	2.21	0.40
1:D:98:ALA:HB1	1:D:129:VAL:CG1	2.51	0.40
1:B:43:HIS:HD2	1:B:44:GLU:N	2.19	0.40
1:A:64:SER:HB2	1:A:66:ASP:OD1	2.21	0.40
1:C:225:VAL:HG12	1:C:225:VAL:O	2.21	0.40
1:D:98:ALA:O	1:D:101:ILE:HG13	2.21	0.40
1:D:189:ASP:O	1:D:190:ASN:CB	2.70	0.40
1:D:152:LYS:HA	1:D:152:LYS:CE	2.43	0.40
1:D:49:LEU:HD11	1:D:90:THR:HG23	2.03	0.40
1:D:33:ILE:O	1:D:37:SER:HB3	2.21	0.40
1:C:163:ASP:CG	3:C:303:SAH:HG1	2.42	0.40
1:A:206:ARG:HE	1:A:206:ARG:CA	2.35	0.40
1:D:76:LYS:C	1:D:78:ILE:H	2.24	0.40
1:A:223:LEU:HA	1:A:223:LEU:HD12	1.89	0.40
1:A:165:ASP:O	1:A:166:LYS:CB	2.43	0.40
1:C:168:ASN:HB3	1:C:172:TYR:CE2	2.56	0.40
1:B:200:PRO:N	1:B:201:PRO:CD	2.85	0.40
1:B:202:ASP:C	1:B:204:PRO:HD2	2.41	0.40
1:C:120:GLY:C	1:C:122:PRO:CD	2.87	0.40
1:D:170:LEU:HD12	1:D:218:GLU:CG	2.49	0.40
1:D:92:TYR:C	1:D:94:LEU:H	2.24	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	225/247 (91%)	195 (87%)	19 (8%)	11 (5%)	3	5
1	B	225/247 (91%)	197 (88%)	20 (9%)	8 (4%)	4	9
1	C	225/247 (91%)	176 (78%)	28 (12%)	21 (9%)	1	1
1	D	225/247 (91%)	157 (70%)	45 (20%)	23 (10%)	1	0
All	All	900/988 (91%)	725 (81%)	112 (12%)	63 (7%)	1	2

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	TYR
1	A	165	ASP
1	A	202	ASP
1	A	231	ILE
1	B	166	LYS
1	B	204	PRO
1	B	231	ILE
1	C	110	MET
1	C	112	ILE
1	C	182	VAL
1	C	184	GLY
1	C	201	PRO
1	C	202	ASP
1	C	231	ILE
1	D	181	LYS
1	D	185	VAL
1	D	231	ILE
1	A	44	GLU
1	A	114	LYS
1	A	166	LYS
1	B	63	THR
1	B	89	TYR
1	B	202	ASP
1	C	105	GLY
1	C	111	ASP
1	C	152	LYS
1	C	166	LYS
1	C	196	SER
1	D	37	SER
1	D	42	GLU
1	D	102	PRO
1	D	123	VAL
1	D	129	VAL

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Mol	Chain	Res	Type
1	D	153	ASN
1	D	182	VAL
1	A	43	HIS
1	B	193	TRP
1	C	109	ALA
1	C	139	PRO
1	C	200	PRO
1	D	41	ARG
1	D	89	TYR
1	D	193	TRP
1	D	232	CYS
1	C	104	ASP
1	C	165	ASP
1	C	185	VAL
1	C	197	VAL
1	D	186	ILE
1	D	194	ASN
1	D	201	PRO
1	A	185	VAL
1	A	204	PRO
1	C	88	VAL
1	B	62	THR
1	D	79	ASN
1	D	200	PRO
1	C	129	VAL
1	D	88	VAL
1	D	199	ALA
1	D	235	PRO
1	D	124	ILE
1	A	201	PRO

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	196/214 (92%)	174 (89%)	22 (11%)	7 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	196/214 (92%)	180 (92%)	16 (8%)	14	32
1	C	196/214 (92%)	179 (91%)	17 (9%)	13	29
1	D	192/214 (90%)	178 (93%)	14 (7%)	17	39
All	All	780/856 (91%)	711 (91%)	69 (9%)	12	28

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	69	GLN
1	A	79	ASN
1	A	90	THR
1	A	94	LEU
1	A	95	LEU
1	A	115	GLU
1	A	136	ARG
1	A	141	LEU
1	A	166	LYS
1	A	170	LEU
1	A	175	ARG
1	A	176	LEU
1	A	180	VAL
1	A	205	LEU
1	A	206	ARG
1	A	209	VAL
1	A	219	LEU
1	A	223	LEU
1	A	230	GLU
1	A	231	ILE
1	A	240	ILE
1	B	25	GLN
1	B	58	TRP
1	B	69	GLN
1	B	74	LEU
1	B	94	LEU
1	B	95	LEU
1	B	103	GLU
1	B	144	LEU
1	B	165	ASP
1	B	166	LYS
1	B	170	LEU

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Mol	Chain	Res	Type
1	B	176	LEU
1	B	179	LEU
1	B	180	VAL
1	B	185	VAL
1	B	204	PRO
1	C	27	ASP
1	C	61	MET
1	C	74	LEU
1	C	79	ASN
1	C	83	THR
1	C	95	LEU
1	C	103	GLU
1	C	108	LEU
1	C	139	PRO
1	C	152	LYS
1	C	153	ASN
1	C	167	ASP
1	C	170	LEU
1	C	174	LYS
1	C	177	ILE
1	C	180	VAL
1	C	223	LEU
1	D	29	LEU
1	D	41	ARG
1	D	42	GLU
1	D	66	ASP
1	D	73	MET
1	D	136	ARG
1	D	137	GLU
1	D	153	ASN
1	D	167	ASP
1	D	174	LYS
1	D	177	ILE
1	D	194	ASN
1	D	210	ARG
1	D	245	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	31	GLN

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Mol	Chain	Res	Type
1	B	43	HIS
1	B	116	ASN
1	C	43	HIS
1	C	69	GLN
1	C	79	ASN
1	C	113	ASN
1	C	116	ASN
1	C	153	ASN
1	C	168	ASN
1	D	31	GLN
1	D	69	GLN
1	D	116	ASN
1	D	153	ASN
1	D	190	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SAH	A	301	-	20,28,28	1.72	4 (20%)	19,40,40	3.62	12 (63%)
4	SPF	A	401	-	56,67,67	11.35	18 (32%)	66,102,102	3.62	26 (39%)
3	SAH	B	302	-	20,28,28	1.52	3 (15%)	19,40,40	3.05	10 (52%)
3	SAH	C	303	-	20,28,28	1.68	3 (15%)	19,40,40	2.94	10 (52%)
3	SAH	D	304	-	20,28,28	1.75	3 (15%)	19,40,40	3.20	8 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	A	301	-	-	0/7/31/31	0/3/3/3
4	SPF	A	401	-	1/1/13/17	0/44/88/88	0/4/5/5
3	SAH	B	302	-	-	0/7/31/31	0/3/3/3
3	SAH	C	303	-	-	0/7/31/31	0/3/3/3
3	SAH	D	304	-	-	0/7/31/31	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	SPF	C2P-S1P	-5.43	1.57	1.81
4	A	401	SPF	P2A-O6A	-4.35	1.48	1.60
4	A	401	SPF	O5B-C5B	-4.05	1.28	1.44
3	C	303	SAH	C8-N7	-3.61	1.27	1.34
3	D	304	SAH	C8-N7	-3.45	1.28	1.34
4	A	401	SPF	C2-C1	-3.42	1.35	1.40
3	B	302	SAH	C8-N7	-3.37	1.28	1.34
3	A	301	SAH	C8-N7	-3.18	1.28	1.34
3	A	301	SAH	O2'-C2'	-2.38	1.37	1.43
4	A	401	SPF	P1A-O1A	-2.35	1.44	1.54
3	A	301	SAH	C5-C4	-2.35	1.35	1.40
3	C	303	SAH	O2'-C2'	-2.32	1.37	1.43
3	B	302	SAH	O2'-C2'	-2.27	1.37	1.43
4	A	401	SPF	O4B-C1B	-2.25	1.38	1.41
3	D	304	SAH	O2'-C2'	-2.18	1.37	1.43
4	A	401	SPF	C5P-N4P	-2.11	1.28	1.33
4	A	401	SPF	C9P-N8P	2.01	1.38	1.34
4	A	401	SPF	O13-C6	2.12	1.40	1.37
4	A	401	SPF	C7P-C6P	2.55	1.59	1.51
3	B	302	SAH	O4'-C1'	4.14	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	SPF	O9P-C9P	4.73	1.31	1.22
4	A	401	SPF	C3P-N4P	4.74	1.57	1.46
3	A	301	SAH	O4'-C1'	4.84	1.47	1.41
3	C	303	SAH	O4'-C1'	5.16	1.47	1.41
3	D	304	SAH	O4'-C1'	5.56	1.48	1.41
4	A	401	SPF	C6-C1	6.13	1.48	1.40
4	A	401	SPF	C7P-N8P	6.17	1.60	1.46
4	A	401	SPF	C2P-C3P	6.49	1.77	1.51
4	A	401	SPF	C5-C6	7.56	1.52	1.38
4	A	401	SPF	CAP-C9P	13.10	1.64	1.53
4	A	401	SPF	CAP-CCP	81.75	2.34	1.47

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	SPF	C2P-C3P-N4P	-9.02	94.31	112.36
3	A	301	SAH	C4'-O4'-C1'	-8.85	99.99	109.72
3	A	301	SAH	N3-C2-N1	-8.57	122.33	128.89
4	A	401	SPF	O10-C9-S1P	-8.39	111.83	122.37
3	D	304	SAH	N3-C2-N1	-8.16	122.65	128.89
3	B	302	SAH	N3-C2-N1	-7.79	122.93	128.89
3	D	304	SAH	C4'-O4'-C1'	-7.74	101.21	109.72
3	C	303	SAH	N3-C2-N1	-7.53	123.13	128.89
4	A	401	SPF	O5P-C5P-C6P	-5.86	111.88	121.98
4	A	401	SPF	O10-C9-C8	-5.39	102.83	118.37
3	C	303	SAH	C4'-O4'-C1'	-5.39	103.80	109.72
3	B	302	SAH	C4'-O4'-C1'	-5.33	103.86	109.72
4	A	401	SPF	C7P-N8P-C9P	-5.01	115.25	122.06
4	A	401	SPF	C3P-N4P-C5P	-3.92	115.08	122.79
4	A	401	SPF	CEP-CBP-CDP	-3.86	109.02	112.66
4	A	401	SPF	C3-C4-C7	-3.70	108.68	120.59
3	B	302	SAH	O4'-C1'-N9	-3.62	100.52	108.10
4	A	401	SPF	O13-C6-C1	-3.35	111.10	114.47
4	A	401	SPF	C7P-C6P-C5P	-3.16	107.10	112.31
3	C	303	SAH	O4'-C1'-N9	-2.77	102.30	108.10
4	A	401	SPF	P2A-O6A-CCP	-2.59	109.92	119.41
3	A	301	SAH	O4'-C4'-C3'	-2.53	100.05	105.15
4	A	401	SPF	O5P-C5P-N4P	-2.27	118.44	122.94
4	A	401	SPF	C5-C4-C3	-2.22	115.73	119.11
3	D	304	SAH	O4'-C1'-N9	-2.08	103.75	108.10
3	C	303	SAH	O4'-C4'-C3'	-2.03	101.05	105.15
4	A	401	SPF	C4-C5-C6	-2.03	117.49	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	SAH	C4'-C5'-SD	2.27	120.52	113.53
3	A	301	SAH	N6-C6-N1	2.30	124.15	119.20
3	D	304	SAH	O4'-C4'-C5'	2.38	115.34	108.85
3	A	301	SAH	C4'-C5'-SD	2.45	121.10	113.53
3	C	303	SAH	C5'-C4'-C3'	2.46	121.35	114.98
3	A	301	SAH	C5'-C4'-C3'	2.48	121.40	114.98
3	B	302	SAH	C2'-C1'-N9	2.52	118.14	114.29
3	D	304	SAH	N6-C6-N1	2.56	124.70	119.20
3	C	303	SAH	N6-C6-N1	2.61	124.80	119.20
3	B	302	SAH	C5'-C4'-C3'	2.73	122.05	114.98
3	B	302	SAH	N6-C6-N1	2.73	125.06	119.20
3	C	303	SAH	C1'-N9-C4	2.77	131.12	126.94
3	A	301	SAH	O4'-C4'-C5'	2.79	116.45	108.85
4	A	401	SPF	O3A-P1A-O5B	2.84	110.48	102.94
4	A	401	SPF	C6P-C7P-N8P	2.92	118.29	111.88
4	A	401	SPF	O13-C6-C5	3.00	129.34	124.21
4	A	401	SPF	O11-C2-C1	3.03	117.52	114.47
3	A	301	SAH	CB-CG-SD	3.15	119.65	113.57
3	B	302	SAH	O2'-C2'-C3'	3.15	122.09	111.83
3	A	301	SAH	C4-C5-N7	3.18	112.40	109.48
3	C	303	SAH	O2'-C2'-C3'	3.22	122.29	111.83
3	D	304	SAH	O2'-C2'-C3'	3.22	122.30	111.83
3	A	301	SAH	O2'-C2'-C3'	3.35	122.71	111.83
4	A	401	SPF	O3A-P2A-O6A	3.36	113.31	103.63
3	D	304	SAH	C4-C5-N7	3.52	112.72	109.48
3	B	302	SAH	C2-N1-C6	3.57	125.14	118.77
3	A	301	SAH	C2-N1-C6	3.57	125.15	118.77
3	C	303	SAH	C4-C5-N7	3.60	112.79	109.48
3	C	303	SAH	C2-N1-C6	3.63	125.25	118.77
3	D	304	SAH	C2-N1-C6	3.65	125.29	118.77
3	B	302	SAH	C4-C5-N7	3.78	112.96	109.48
3	A	301	SAH	C2'-C1'-N9	4.13	120.61	114.29
4	A	401	SPF	C5-C4-C7	4.66	135.59	120.59
4	A	401	SPF	O5B-C5B-C4B	5.03	127.67	109.12
4	A	401	SPF	C2P-S1P-C9	5.34	106.38	99.59
4	A	401	SPF	C6P-C5P-N4P	5.60	126.18	116.46
4	A	401	SPF	C4-C3-C2	6.40	128.63	120.17
4	A	401	SPF	C11-O11-C2	8.92	131.07	117.54
4	A	401	SPF	C7-C8-C9	15.18	146.79	121.81

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	401	SPF	C2B

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	SAH	4	0
4	A	401	SPF	23	0
3	B	302	SAH	2	0
3	C	303	SAH	6	0
3	D	304	SAH	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	227/247 (91%)	-0.05	6 (2%) 59 59	33, 47, 70, 96	0
1	B	227/247 (91%)	0.10	12 (5%) 30 28	33, 48, 74, 94	0
1	C	227/247 (91%)	0.44	20 (8%) 12 10	44, 72, 105, 115	0
1	D	227/247 (91%)	1.11	45 (19%) 1 1	76, 110, 130, 138	0
All	All	908/988 (91%)	0.40	83 (9%) 11 9	33, 62, 124, 138	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	ALA	8.1
1	C	200	PRO	6.3
1	C	201	PRO	5.7
1	C	111	ASP	5.2
1	D	246	ILE	5.1
1	B	202	ASP	5.1
1	D	104	ASP	4.7
1	B	201	PRO	4.2
1	C	110	MET	4.2
1	B	62	THR	4.1
1	D	152	LYS	4.0
1	B	204	PRO	4.0
1	D	151	GLU	3.9
1	D	48	GLU	3.9
1	D	134	ASP	3.8
1	D	103	GLU	3.7
1	D	161	PHE	3.7
1	D	41	ARG	3.7
1	C	151	GLU	3.6
1	D	102	PRO	3.5
1	D	201	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	247	LYS	3.4
1	D	80	ALA	3.4
1	D	85	GLU	3.4
1	D	162	VAL	3.3
1	D	27	ASP	3.3
1	C	247	LYS	3.2
1	D	188	TYR	3.2
1	C	202	ASP	3.2
1	B	63	THR	3.1
1	D	52	VAL	3.1
1	D	105	GLY	3.0
1	D	84	MET	2.9
1	D	86	ILE	2.9
1	C	61	MET	2.8
1	A	161	PHE	2.8
1	B	198	VAL	2.8
1	D	81	LYS	2.7
1	D	79	ASN	2.7
1	B	187	GLY	2.7
1	D	125	LYS	2.7
1	C	162	VAL	2.7
1	C	86	ILE	2.6
1	C	161	PHE	2.6
1	D	29	LEU	2.6
1	C	182	VAL	2.6
1	D	51	GLU	2.6
1	D	187	GLY	2.5
1	C	60	ILE	2.5
1	A	240	ILE	2.5
1	B	162	VAL	2.4
1	D	206	ARG	2.4
1	A	206	ARG	2.4
1	B	195	GLY	2.4
1	D	43	HIS	2.4
1	C	149	LYS	2.3
1	D	108	LEU	2.3
1	C	83	THR	2.3
1	D	56	HIS	2.3
1	C	160	ILE	2.3
1	D	150	ASP	2.3
1	D	30	TYR	2.3
1	A	204	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	149	LYS	2.2
1	D	163	ASP	2.2
1	D	181	LYS	2.2
1	D	240	ILE	2.2
1	D	126	LYS	2.2
1	C	85	GLU	2.2
1	D	208	TYR	2.1
1	A	202	ASP	2.1
1	C	106	LYS	2.1
1	D	44	GLU	2.1
1	D	87	GLY	2.1
1	D	149	LYS	2.1
1	B	150	ASP	2.1
1	D	109	ALA	2.1
1	D	118	GLU	2.0
1	A	103	GLU	2.0
1	C	103	GLU	2.0
1	D	129	VAL	2.0
1	D	186	ILE	2.0
1	C	109	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	SPF	A	401	63/63	0.35	0.80	7.93	176,192,195,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SAH	C	303	26/26	0.20	0.76	5.40	159,170,171,171	0
2	CA	B	306	1/1	0.94	0.27	3.36	121,121,121,121	0
3	SAH	B	302	26/26	0.61	0.42	2.94	109,119,122,122	0
3	SAH	D	304	26/26	0.68	0.32	0.98	130,135,139,139	0
2	CA	D	308	1/1	0.96	0.28	0.69	87,87,87,87	0
3	SAH	A	301	26/26	0.93	0.23	0.41	37,47,56,57	0
2	CA	A	305	1/1	0.94	0.31	-	54,54,54,54	0
2	CA	C	307	1/1	0.97	0.16	-	59,59,59,59	0

6.5 Other polymers

There are no such residues in this entry.