Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 02:00 AM GMT

PDB ID	:	3IL4
Title	:	Structure of E. faecalis FabH in complex with acetyl CoA
Authors	:	Gajiwala, K.S.; Margosiak, S; Lu, J.; Cortez, J.; Su, Y.; Nie, Z.; Appelt, K.
Deposited on	:	2009-08-06
Resolution	:	3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html

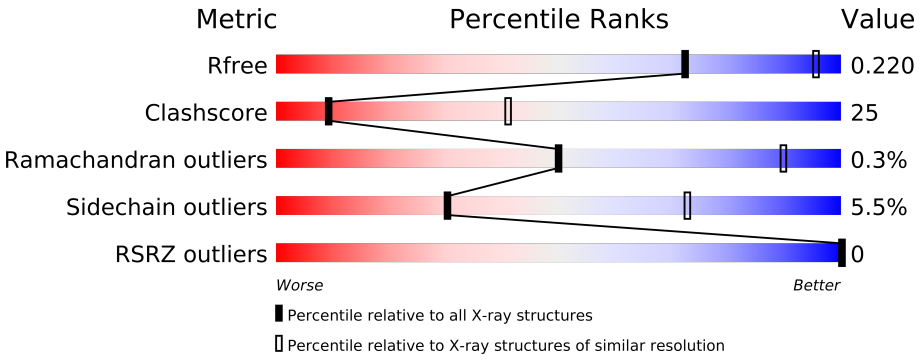
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	320	
1	B	320	
1	C	320	
1	D	320	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ACO	B	401	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10031 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

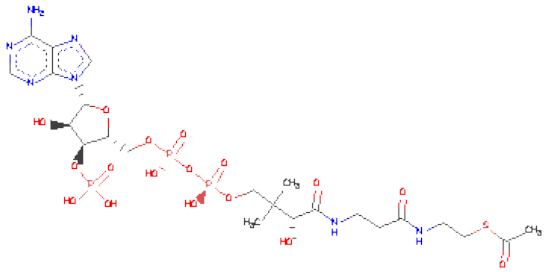
- Molecule 1 is a protein called 3-oxoacyl-[acyl-carrier-protein]synthase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2450	1540	415	483	12			
1	B	317	Total	C	N	O	S	0	0	0
			2441	1534	413	482	12			
1	C	317	Total	C	N	O	S	0	0	0
			2441	1534	413	482	12			
1	D	318	Total	C	N	O	S	0	0	0
			2450	1540	415	483	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	THR	ALA	ENGINEERED	UNP Q820T1
A	253	SER	ASN	ENGINEERED	UNP Q820T1
B	192	THR	ALA	ENGINEERED	UNP Q820T1
B	253	SER	ASN	ENGINEERED	UNP Q820T1
C	192	THR	ALA	ENGINEERED	UNP Q820T1
C	253	SER	ASN	ENGINEERED	UNP Q820T1
D	192	THR	ALA	ENGINEERED	UNP Q820T1
D	253	SER	ASN	ENGINEERED	UNP Q820T1

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is water.

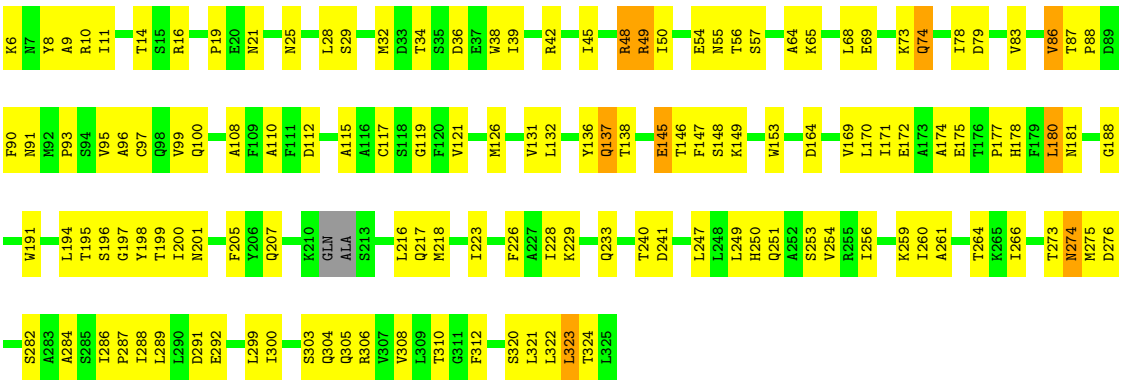
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	12	Total	O	0	0
			12	12		
3	C	7	Total	O	0	0
			7	7		
3	D	15	Total	O	0	0
			15	15		

3 Residue-property plots (i)

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

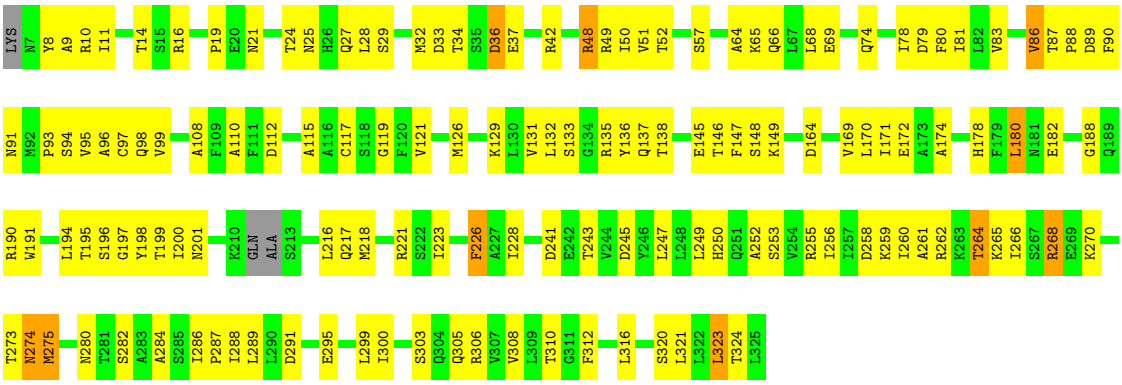
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein]synthase 3

Chain A:



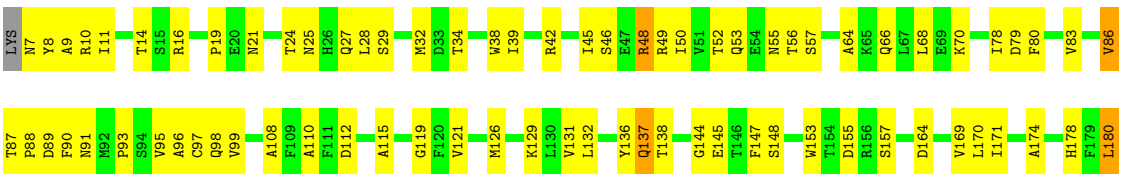
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein]synthase 3

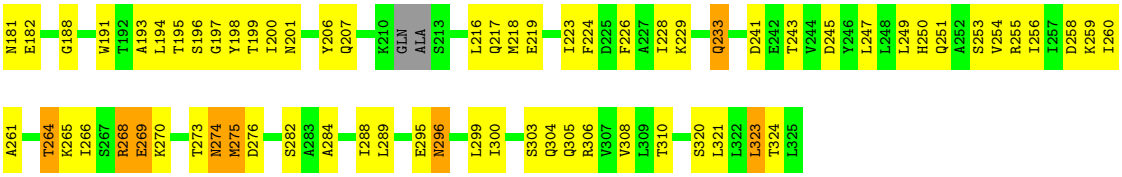
Chain B:



• Molecule 1: 3-oxoacyl-[acyl-carrier-protein]synthase 3

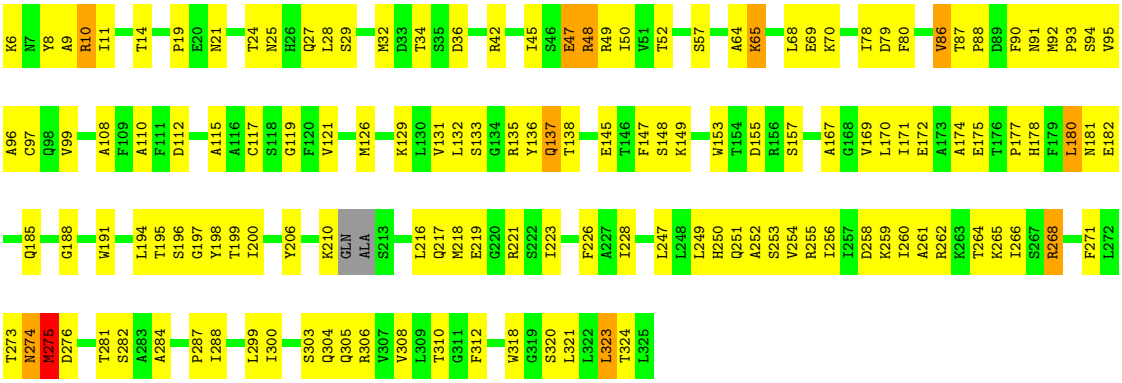
Chain C:





• Molecule 1: 3-oxoacyl-[acyl-carrier-protein]synthase 3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.75Å 93.30Å 104.25Å 90.00° 93.90° 90.00°	Depositor
Resolution (Å)	24.88 – 3.00 24.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (24.88-3.00) 97.2 (24.88-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 2.99Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, R_{free}	0.196 , 0.270 0.191 , 0.220	Depositor DCC
R_{free} test set	2471 reflections (10.99%)	DCC
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.979	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 16.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 25389 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10031	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, ACO

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	0.41	0/2473	0.65	0/3342
1	B	0.40	0/2464	0.66	0/3331
1	C	0.40	0/2464	0.67	0/3331
1	D	0.40	0/2473	0.66	0/3342
All	All	0.41	0/9874	0.66	0/13346

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2450	0	2431	125	0
1	B	2441	0	2418	136	0
1	C	2441	0	2418	147	0
1	D	2450	0	2431	122	0
2	A	51	0	33	1	0
2	B	51	0	34	1	0
2	C	51	0	33	3	0
2	D	51	0	34	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	11	0	0	2	0
3	B	12	0	0	2	0
3	C	7	0	0	1	0
3	D	15	0	0	5	0
All	All	10031	0	9832	491	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (491) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:10:ARG:HD3	1:B:174:ALA:HB2	1.30	1.12
1:C:42:ARG:NH2	1:C:255:ARG:HH12	1.58	0.99
1:C:10:ARG:HD3	1:C:174:ALA:HB2	1.47	0.95
1:A:10:ARG:HD3	1:A:174:ALA:HB2	1.55	0.88
1:C:42:ARG:HE	1:C:255:ARG:NH2	1.72	0.88
1:B:249:LEU:HG	1:B:310:THR:OG1	1.79	0.83
1:C:42:ARG:HH21	1:C:255:ARG:HH12	1.23	0.81
1:A:198:TYR:HE2	1:A:200:ILE:HG22	1.44	0.81
1:C:42:ARG:HE	1:C:255:ARG:CZ	1.92	0.81
1:A:249:LEU:HG	1:A:310:THR:OG1	1.82	0.80
1:D:249:LEU:HG	1:D:310:THR:OG1	1.81	0.80
1:C:91:ASN:ND2	1:D:197:GLY:HA3	1.96	0.80
1:C:198:TYR:HE2	1:C:200:ILE:HG22	1.47	0.79
1:B:121:VAL:HG13	1:B:321:LEU:HG	1.65	0.78
1:D:121:VAL:HG13	1:D:321:LEU:HG	1.66	0.78
1:C:249:LEU:HG	1:C:310:THR:OG1	1.83	0.78
1:C:42:ARG:CZ	1:C:255:ARG:HH12	1.96	0.78
1:D:198:TYR:HE2	1:D:200:ILE:HG22	1.48	0.78
1:C:121:VAL:HG13	1:C:321:LEU:HG	1.67	0.76
1:B:198:TYR:HE2	1:B:200:ILE:HG22	1.48	0.76
1:A:121:VAL:HG13	1:A:321:LEU:HG	1.65	0.76
1:D:42:ARG:O	1:D:255:ARG:HD3	1.86	0.75
1:A:228:ILE:HD12	1:A:259:LYS:HB2	1.69	0.74
1:C:38:TRP:O	1:C:42:ARG:HG2	1.87	0.74
1:C:195:THR:HG22	1:D:93:PRO:HD3	1.69	0.74
1:A:93:PRO:HD3	1:B:195:THR:HG22	1.70	0.74
1:A:198:TYR:CE2	1:A:200:ILE:HG22	2.23	0.74
1:A:25:ASN:ND2	1:A:39:ILE:HB	2.02	0.73
1:B:198:TYR:CE2	1:B:200:ILE:HG22	2.24	0.73
1:C:198:TYR:CE2	1:C:200:ILE:HG22	2.23	0.72
1:C:25:ASN:ND2	1:C:39:ILE:HG21	2.03	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:16:ARG:HG2	1:B:291:ASP:OD2	1.89	0.72
1:B:42:ARG:HA	1:B:255:ARG:HD3	1.72	0.71
1:B:228:ILE:HD12	1:B:259:LYS:HB2	1.70	0.71
1:A:25:ASN:HD22	1:A:39:ILE:HB	1.54	0.70
1:C:25:ASN:HD22	1:C:39:ILE:CD1	2.04	0.70
1:C:303:SER:OG	1:C:305:GLN:HG3	1.91	0.70
1:D:198:TYR:CE2	1:D:200:ILE:HG22	2.25	0.70
1:C:96:ALA:HB1	1:C:110:ALA:HB1	1.74	0.70
1:B:261:ALA:O	1:B:264:THR:HG22	1.91	0.70
1:B:264:THR:HG23	1:B:266:ILE:H	1.57	0.70
1:C:261:ALA:O	1:C:264:THR:HG22	1.92	0.69
1:A:25:ASN:OD1	1:A:48:ARG:NH2	2.26	0.69
1:D:261:ALA:O	1:D:264:THR:HG22	1.94	0.68
1:D:96:ALA:HB1	1:D:110:ALA:HB1	1.74	0.68
1:A:261:ALA:O	1:A:264:THR:HG22	1.95	0.67
1:C:273:THR:HG23	1:C:275:MET:SD	2.34	0.67
1:C:25:ASN:HD21	1:C:39:ILE:HG21	1.59	0.67
1:A:96:ALA:HB1	1:A:110:ALA:HB1	1.76	0.67
1:D:273:THR:HG23	1:D:275:MET:SD	2.35	0.67
1:B:303:SER:OG	1:B:305:GLN:HG3	1.94	0.67
1:B:19:PRO:HD2	1:B:49:ARG:HB3	1.76	0.67
1:B:10:ARG:HD3	1:B:174:ALA:CB	2.19	0.67
1:C:178:HIS:HA	1:C:324:THR:CG2	2.24	0.66
1:A:273:THR:HG23	1:A:275:MET:SD	2.35	0.66
1:B:245:ASP:OD2	1:B:306:ARG:HG3	1.95	0.66
1:B:273:THR:HG23	1:B:275:MET:SD	2.35	0.66
1:B:178:HIS:HA	1:B:324:THR:CG2	2.26	0.66
1:D:216:LEU:HD23	1:D:217:GLN:N	2.11	0.65
1:B:96:ALA:HB1	1:B:110:ALA:HB1	1.76	0.65
1:C:25:ASN:HD22	1:C:39:ILE:HD12	1.61	0.65
1:A:195:THR:HG22	1:B:93:PRO:HD3	1.79	0.65
1:A:145:GLU:HG2	1:A:147:PHE:CE2	2.32	0.65
1:B:274:ASN:HB2	1:B:289:LEU:HD13	1.77	0.65
1:A:178:HIS:HA	1:A:324:THR:CG2	2.28	0.64
1:A:91:ASN:ND2	1:B:197:GLY:HA3	2.12	0.64
1:C:42:ARG:NE	1:C:255:ARG:NH1	2.46	0.64
1:D:268:ARG:HE	1:D:271:PHE:HB2	1.62	0.64
1:C:25:ASN:ND2	1:C:48:ARG:HH22	1.95	0.64
1:A:126:MET:SD	1:B:126:MET:SD	2.96	0.64
1:C:42:ARG:HG3	1:C:42:ARG:HH11	1.62	0.64
1:D:178:HIS:HA	1:D:324:THR:CG2	2.28	0.64
1:D:6:LYS:N	3:D:5:HOH:O	2.30	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:264:THR:HG23	1:C:266:ILE:H	1.63	0.63
1:C:229:LYS:O	1:C:233:GLN:HG2	1.98	0.63
1:A:79:ASP:HB2	1:A:138:THR:O	2.00	0.62
1:D:206:TYR:OH	1:D:210:LYS:HG3	1.99	0.62
1:A:207:GLN:HG2	1:B:52:THR:HB	1.80	0.62
1:C:269:GLU:N	1:C:269:GLU:OE1	2.33	0.62
1:D:303:SER:O	1:D:304:GLN:HB2	1.98	0.61
1:B:216:LEU:HD23	1:B:217:GLN:N	2.15	0.61
1:B:299:LEU:HA	1:B:305:GLN:HE22	1.65	0.61
1:B:25:ASN:HD21	1:B:48:ARG:HH12	1.49	0.61
1:D:178:HIS:O	1:D:180:LEU:HD13	1.99	0.61
1:B:21:ASN:HB3	1:B:50:ILE:O	2.00	0.61
1:B:178:HIS:O	1:B:180:LEU:HD13	2.01	0.61
1:D:323:LEU:O	1:D:323:LEU:HD12	2.01	0.61
1:C:323:LEU:HD12	1:C:323:LEU:O	2.00	0.60
1:D:133:SER:OG	1:D:135:ARG:HG3	2.02	0.60
1:A:223:ILE:HG21	2:A:401:ACO:HH32	1.83	0.60
1:B:300:ILE:H	1:B:305:GLN:NE2	1.99	0.60
1:D:155:ASP:OD2	1:D:157:SER:HB2	2.01	0.60
1:B:37:GLU:HA	1:B:37:GLU:OE2	2.01	0.60
1:C:42:ARG:HE	1:C:255:ARG:NH1	1.99	0.59
1:A:8:TYR:O	1:A:174:ALA:N	2.33	0.59
1:B:252:ALA:HB1	2:B:401:ACO:H22	1.84	0.59
1:C:216:LEU:HD23	1:C:217:GLN:N	2.17	0.59
1:B:8:TYR:O	1:B:174:ALA:N	2.32	0.59
1:D:228:ILE:HD12	1:D:259:LYS:HB2	1.83	0.59
1:C:42:ARG:HH21	1:C:255:ARG:NH1	1.99	0.59
1:C:25:ASN:OD1	1:C:46:SER:HA	2.03	0.59
1:B:323:LEU:O	1:B:323:LEU:HD12	2.03	0.59
1:C:178:HIS:O	1:C:180:LEU:HD13	2.03	0.58
1:C:233:GLN:HA	1:C:233:GLN:HE21	1.66	0.58
1:B:145:GLU:HG2	1:B:147:PHE:CE2	2.38	0.58
1:D:223:ILE:HG21	2:D:401:ACO:HH32	1.86	0.58
1:C:243:THR:O	1:C:306:ARG:HD3	2.04	0.58
1:C:89:ASP:HB2	1:C:98:GLN:HE22	1.68	0.58
1:C:24:THR:OG1	1:C:27:GLN:HG3	2.03	0.58
1:C:93:PRO:HD3	1:D:195:THR:HG22	1.85	0.58
1:D:181:ASN:OD1	1:D:182:GLU:N	2.36	0.57
1:C:25:ASN:ND2	1:C:39:ILE:CG2	2.66	0.57
1:C:126:MET:SD	1:D:126:MET:SD	3.03	0.57
1:B:260:ILE:O	1:B:264:THR:HB	2.05	0.57
1:B:221:ARG:HG3	1:B:221:ARG:HH21	1.70	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:42:ARG:CZ	1:C:255:ARG:NH1	2.68	0.57
1:B:228:ILE:HD12	1:B:259:LYS:CB	2.34	0.56
1:C:191:TRP:HB2	1:D:93:PRO:HG3	1.86	0.56
1:A:323:LEU:O	1:A:323:LEU:HD12	2.05	0.56
1:A:300:ILE:H	1:A:305:GLN:HE22	1.52	0.56
1:A:38:TRP:O	1:A:42:ARG:HG2	2.05	0.56
1:D:78:ILE:O	1:D:108:ALA:HB2	2.05	0.56
1:A:9:ALA:HB1	1:A:171:ILE:HD11	1.88	0.56
1:C:9:ALA:HB1	1:C:171:ILE:HD11	1.88	0.56
1:C:42:ARG:HE	1:C:255:ARG:HH22	1.51	0.56
1:B:79:ASP:HB2	1:B:138:THR:O	2.05	0.56
1:A:178:HIS:O	1:A:180:LEU:HD13	2.05	0.56
1:D:9:ALA:HB1	1:D:171:ILE:HD11	1.87	0.55
1:A:306:ARG:NH2	1:A:322:LEU:HD21	2.21	0.55
1:B:264:THR:HG23	1:B:266:ILE:N	2.21	0.55
1:A:50:ILE:HG23	1:A:148:SER:HB3	1.87	0.55
1:B:250:HIS:NE2	1:B:280:ASN:ND2	2.54	0.55
1:C:197:GLY:HA3	1:D:91:ASN:HD22	1.71	0.55
1:B:243:THR:HB	1:B:306:ARG:NH2	2.22	0.55
1:B:252:ALA:HA	1:B:280:ASN:HD22	1.71	0.55
1:A:65:LYS:O	1:A:69:GLU:HG3	2.07	0.55
1:D:185:GLN:NE2	1:D:318:TRP:CZ2	2.75	0.55
1:D:221:ARG:HH11	2:D:401:ACO:H132	1.70	0.54
1:C:197:GLY:HA3	1:D:91:ASN:ND2	2.22	0.54
1:D:219:GLU:HB3	3:D:328:HOH:O	2.07	0.54
1:B:78:ILE:O	1:B:108:ALA:HB2	2.07	0.54
1:D:50:ILE:HG23	1:D:148:SER:HB3	1.89	0.54
1:A:241:ASP:HB2	1:A:266:ILE:HA	1.90	0.54
1:B:24:THR:OG1	1:B:27:GLN:HG3	2.07	0.54
1:A:93:PRO:HG3	1:B:191:TRP:HB2	1.89	0.54
1:D:284:ALA:O	1:D:288:ILE:HG13	2.08	0.54
1:D:137:GLN:N	1:D:137:GLN:NE2	2.55	0.54
1:C:8:TYR:O	1:C:174:ALA:N	2.37	0.54
1:D:260:ILE:O	1:D:264:THR:HB	2.08	0.54
1:A:16:ARG:HG2	1:A:291:ASP:OD2	2.08	0.54
1:B:65:LYS:O	1:B:69:GLU:HG3	2.07	0.54
1:C:264:THR:HG23	1:C:266:ILE:N	2.22	0.53
1:B:9:ALA:HB1	1:B:171:ILE:HD11	1.90	0.53
1:C:284:ALA:O	1:C:288:ILE:HG13	2.07	0.53
1:B:25:ASN:ND2	1:B:48:ARG:HH12	2.06	0.53
1:C:25:ASN:ND2	1:C:48:ARG:NH2	2.56	0.53
1:B:250:HIS:CE1	1:B:282:SER:HA	2.44	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:25:ASN:HD21	1:C:39:ILE:CG2	2.20	0.53
1:B:25:ASN:HD22	1:B:48:ARG:HH22	1.57	0.53
1:B:51:VAL:HG22	1:B:164:ASP:OD2	2.08	0.53
1:C:310:THR:HG22	1:C:320:SER:CB	2.38	0.53
1:C:260:ILE:O	1:C:264:THR:HB	2.09	0.53
1:C:93:PRO:HG3	1:D:191:TRP:HB2	1.90	0.53
1:A:83:VAL:O	1:A:112:ASP:HA	2.09	0.53
1:C:181:ASN:OD1	1:D:135:ARG:NH1	2.41	0.53
1:C:50:ILE:HG23	1:C:148:SER:HB3	1.90	0.53
1:D:8:TYR:O	1:D:174:ALA:N	2.36	0.53
1:C:250:HIS:CE1	1:C:282:SER:HA	2.44	0.53
1:C:251:GLN:NE2	1:C:289:LEU:HD22	2.24	0.53
1:A:250:HIS:CE1	1:A:282:SER:HA	2.43	0.53
1:A:45:ILE:HA	1:A:276:ASP:HA	1.90	0.53
1:A:229:LYS:O	1:A:233:GLN:HG2	2.08	0.53
1:C:79:ASP:HB2	1:C:138:THR:O	2.08	0.53
1:A:188:GLY:O	1:A:191:TRP:HD1	1.92	0.53
1:A:131:VAL:HA	1:A:136:TYR:O	2.09	0.52
1:A:303:SER:O	1:A:304:GLN:HB2	2.09	0.52
1:C:16:ARG:NH1	1:C:295:GLU:OE2	2.42	0.52
1:D:216:LEU:HD23	1:D:216:LEU:C	2.30	0.52
1:B:11:ILE:HG23	1:B:169:VAL:HB	1.91	0.52
1:D:299:LEU:HD23	1:D:305:GLN:NE2	2.25	0.52
1:B:50:ILE:HG23	1:B:148:SER:HB3	1.89	0.52
1:C:274:ASN:HB2	1:C:289:LEU:HD13	1.91	0.52
1:A:90:PHE:HB3	1:B:196:SER:O	2.10	0.52
1:A:310:THR:HG22	1:A:320:SER:CB	2.39	0.52
1:B:25:ASN:HB3	1:B:36:ASP:HA	1.91	0.52
1:A:216:LEU:HD23	1:A:217:GLN:N	2.25	0.52
1:D:250:HIS:CE1	1:D:282:SER:HA	2.44	0.52
1:D:258:ASP:O	1:D:262:ARG:HG3	2.10	0.52
1:D:11:ILE:HG23	1:D:169:VAL:HB	1.92	0.52
1:A:11:ILE:HG23	1:A:169:VAL:HB	1.91	0.52
1:C:228:ILE:HD12	1:C:259:LYS:HB2	1.91	0.52
1:C:42:ARG:NH2	2:C:401:ACO:OAP	2.43	0.51
1:C:241:ASP:O	1:C:270:LYS:NZ	2.42	0.51
1:A:233:GLN:HA	1:A:233:GLN:HE21	1.74	0.51
1:A:201:ASN:ND2	1:B:149:LYS:HB3	2.24	0.51
1:B:87:THR:N	1:B:88:PRO:CD	2.73	0.51
1:B:264:THR:CG2	1:B:266:ILE:H	2.22	0.51
1:B:25:ASN:ND2	1:B:48:ARG:HH22	2.09	0.51
1:D:10:ARG:HG2	1:D:174:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:ASN:OD1	1:B:135:ARG:NH1	2.43	0.51
1:A:87:THR:N	1:A:88:PRO:CD	2.74	0.51
1:A:97:CYS:O	1:B:188:GLY:HA3	2.11	0.51
1:D:25:ASN:HB3	1:D:36:ASP:HA	1.91	0.51
1:A:247:LEU:HG	1:A:308:VAL:CG1	2.40	0.51
1:B:310:THR:HG22	1:B:320:SER:CB	2.41	0.51
1:B:300:ILE:H	1:B:305:GLN:HE21	1.57	0.51
1:B:29:SER:HA	1:B:34:THR:HG23	1.92	0.51
1:B:66:GLN:HA	1:B:69:GLU:OE1	2.11	0.51
1:A:197:GLY:HA3	1:B:91:ASN:ND2	2.26	0.51
1:C:129:LYS:HB3	1:D:129:LYS:HB3	1.93	0.51
1:B:188:GLY:O	1:B:191:TRP:HD1	1.94	0.51
1:D:264:THR:HG23	1:D:266:ILE:N	2.26	0.51
1:D:87:THR:N	1:D:88:PRO:CD	2.74	0.51
1:A:284:ALA:O	1:A:288:ILE:HG13	2.09	0.51
1:C:42:ARG:HG3	1:C:42:ARG:NH1	2.25	0.50
1:C:188:GLY:HA3	1:D:97:CYS:O	2.10	0.50
1:C:305:GLN:O	1:C:324:THR:HA	2.12	0.50
1:B:135:ARG:HD2	3:B:331:HOH:O	2.11	0.50
1:C:247:LEU:HG	1:C:308:VAL:CG1	2.42	0.50
1:D:145:GLU:HG3	1:D:281:THR:O	2.11	0.50
1:D:273:THR:CG2	3:D:331:HOH:O	2.59	0.50
1:A:250:HIS:HE1	1:A:282:SER:HA	1.76	0.50
1:A:264:THR:HG23	1:A:266:ILE:N	2.27	0.50
1:C:269:GLU:CD	1:C:269:GLU:H	2.15	0.50
1:C:55:ASN:OD1	1:C:56:THR:N	2.45	0.50
1:C:68:LEU:N	1:C:68:LEU:HD12	2.27	0.50
1:D:65:LYS:HE2	1:D:69:GLU:OE2	2.12	0.50
1:C:87:THR:N	1:C:88:PRO:CD	2.74	0.50
1:C:42:ARG:NE	1:C:255:ARG:HH12	2.09	0.50
1:C:304:GLN:NE2	1:C:324:THR:OG1	2.45	0.50
1:C:264:THR:HG23	1:C:266:ILE:HG13	1.94	0.50
1:A:91:ASN:HD22	1:B:197:GLY:HA3	1.76	0.50
1:D:223:ILE:CG2	2:D:401:ACO:HH32	2.41	0.50
1:C:50:ILE:HA	1:C:164:ASP:OD2	2.12	0.50
1:A:233:GLN:HA	1:A:233:GLN:NE2	2.26	0.50
1:B:14:THR:HG22	1:B:169:VAL:HG12	1.93	0.50
1:C:38:TRP:CZ2	1:C:42:ARG:NH1	2.80	0.49
1:D:310:THR:HG22	1:D:320:SER:CB	2.42	0.49
1:B:94:SER:HB2	1:B:112:ASP:OD1	2.12	0.49
1:B:194:LEU:HB2	1:B:223:ILE:HD11	1.94	0.49
1:B:131:VAL:HA	1:B:136:TYR:O	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:216:LEU:C	1:C:216:LEU:HD23	2.32	0.49
1:B:95:VAL:O	1:B:99:VAL:HG23	2.12	0.49
1:B:241:ASP:O	1:B:270:LYS:NZ	2.45	0.49
1:D:24:THR:HA	1:D:47:GLU:HB3	1.93	0.49
1:B:182:GLU:HB2	1:B:321:LEU:HD23	1.93	0.49
1:D:264:THR:HG23	1:D:266:ILE:HG13	1.94	0.49
1:A:260:ILE:O	1:A:264:THR:HB	2.12	0.49
1:A:194:LEU:HB2	1:A:223:ILE:HD11	1.95	0.49
1:D:194:LEU:HB2	1:D:223:ILE:HD11	1.94	0.49
1:B:221:ARG:NH2	1:B:221:ARG:HG3	2.27	0.49
1:A:216:LEU:HD23	1:A:216:LEU:C	2.33	0.49
1:A:218:MET:SD	1:A:223:ILE:HD12	2.53	0.49
1:C:196:SER:O	1:D:90:PHE:HB3	2.12	0.49
1:A:146:THR:O	1:A:149:LYS:HG2	2.12	0.49
1:C:178:HIS:HA	1:C:324:THR:HG22	1.94	0.49
1:C:250:HIS:HE1	1:C:282:SER:HA	1.78	0.49
1:A:240:THR:O	1:A:241:ASP:C	2.50	0.48
1:B:94:SER:O	1:B:98:GLN:HG3	2.13	0.48
1:C:78:ILE:O	1:C:108:ALA:HB2	2.13	0.48
1:B:284:ALA:O	1:B:288:ILE:HG13	2.13	0.48
1:C:132:LEU:C	1:C:132:LEU:HD23	2.33	0.48
1:A:178:HIS:HA	1:A:324:THR:HG22	1.95	0.48
1:C:145:GLU:OE2	1:C:282:SER:HB3	2.13	0.48
1:D:14:THR:HG22	1:D:169:VAL:HG12	1.94	0.48
1:A:274:ASN:HB3	3:A:327:HOH:O	2.12	0.48
1:A:132:LEU:HD23	1:A:132:LEU:C	2.34	0.48
1:B:247:LEU:HG	1:B:308:VAL:CG1	2.43	0.48
1:C:188:GLY:O	1:C:191:TRP:HD1	1.95	0.48
1:D:194:LEU:HD13	1:D:218:MET:HB3	1.96	0.48
1:C:258:ASP:OD2	1:C:268:ARG:NH2	2.47	0.48
1:B:264:THR:HG23	1:B:266:ILE:HG13	1.94	0.48
1:C:64:ALA:O	1:C:68:LEU:HD13	2.13	0.48
1:C:11:ILE:HG23	1:C:169:VAL:HB	1.94	0.48
1:C:296:ASN:OD1	1:C:296:ASN:C	2.51	0.48
1:A:137:GLN:O	1:A:172:GLU:HA	2.13	0.48
1:A:228:ILE:HD12	1:A:259:LYS:CB	2.41	0.48
1:D:180:LEU:HD23	1:D:306:ARG:HH11	1.79	0.48
1:A:249:LEU:HA	1:A:310:THR:O	2.14	0.48
1:D:250:HIS:HE1	1:D:282:SER:HA	1.79	0.48
1:A:201:ASN:CG	1:B:149:LYS:HB3	2.34	0.48
1:A:149:LYS:HB2	1:B:201:ASN:HA	1.96	0.48
1:B:132:LEU:HD23	1:B:132:LEU:C	2.34	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:216:LEU:C	1:B:216:LEU:HD23	2.34	0.48
1:B:250:HIS:HE1	1:B:282:SER:HA	1.78	0.48
1:D:45:ILE:HA	1:D:276:ASP:HA	1.96	0.48
1:A:196:SER:O	1:B:90:PHE:HB3	2.14	0.47
1:C:299:LEU:C	1:C:300:ILE:HG13	2.35	0.47
1:A:91:ASN:O	1:B:86:VAL:HG22	2.14	0.47
1:D:178:HIS:HA	1:D:324:THR:HG22	1.96	0.47
1:D:131:VAL:HA	1:D:136:TYR:O	2.14	0.47
1:D:68:LEU:N	1:D:68:LEU:HD12	2.29	0.47
1:A:264:THR:HG23	1:A:266:ILE:HG13	1.95	0.47
1:B:133:SER:OG	1:B:135:ARG:HG3	2.14	0.47
1:A:78:ILE:O	1:A:108:ALA:HB2	2.13	0.47
1:C:66:GLN:O	1:C:70:LYS:HB2	2.15	0.47
1:C:182:GLU:HB2	1:C:321:LEU:HD23	1.95	0.47
1:B:178:HIS:HA	1:B:324:THR:HG22	1.96	0.47
1:D:49:ARG:O	1:D:50:ILE:HD13	2.14	0.47
1:B:218:MET:SD	1:B:223:ILE:HD12	2.54	0.47
1:C:264:THR:O	1:C:265:LYS:HB2	2.14	0.47
1:C:323:LEU:HD12	1:C:323:LEU:C	2.35	0.47
1:C:21:ASN:HB3	1:C:50:ILE:O	2.15	0.47
1:A:64:ALA:O	1:A:68:LEU:HD13	2.14	0.47
1:B:19:PRO:O	1:B:49:ARG:NH1	2.45	0.47
1:A:86:VAL:O	1:A:86:VAL:HG13	2.15	0.47
1:C:95:VAL:O	1:C:99:VAL:HG23	2.14	0.47
1:D:132:LEU:HD23	1:D:132:LEU:C	2.34	0.47
1:C:201:ASN:HA	1:D:149:LYS:HB2	1.96	0.47
1:C:131:VAL:HA	1:C:136:TYR:O	2.13	0.47
1:C:42:ARG:NE	1:C:255:ARG:CZ	2.70	0.47
1:D:264:THR:O	1:D:265:LYS:HB2	2.15	0.47
1:D:64:ALA:O	1:D:68:LEU:HD13	2.15	0.47
1:D:253:SER:HB3	1:D:256:ILE:HG13	1.95	0.47
1:A:253:SER:HB3	1:A:256:ILE:HG13	1.96	0.47
1:B:16:ARG:NH2	1:B:295:GLU:OE2	2.30	0.47
1:C:14:THR:HG22	1:C:169:VAL:HG12	1.96	0.47
1:D:95:VAL:O	1:D:99:VAL:HG23	2.15	0.47
1:D:323:LEU:HD12	1:D:323:LEU:C	2.34	0.47
1:C:144:GLY:O	1:C:145:GLU:HG3	2.15	0.47
1:C:19:PRO:HD2	1:C:49:ARG:HB3	1.97	0.47
1:A:25:ASN:ND2	1:A:39:ILE:CB	2.77	0.47
1:A:137:GLN:N	1:A:137:GLN:NE2	2.63	0.47
1:B:258:ASP:HB3	1:B:262:ARG:HH22	1.79	0.47
1:A:29:SER:HA	1:A:34:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:247:LEU:HG	1:D:308:VAL:CG1	2.44	0.47
1:D:29:SER:HA	1:D:34:THR:HG23	1.96	0.47
1:D:264:THR:HG23	1:D:266:ILE:H	1.80	0.46
1:D:218:MET:SD	1:D:223:ILE:HD12	2.55	0.46
1:B:249:LEU:HA	1:B:310:THR:O	2.16	0.46
1:A:191:TRP:HB2	1:B:93:PRO:HG3	1.97	0.46
1:D:299:LEU:C	1:D:300:ILE:HG13	2.36	0.46
1:D:24:THR:OG1	1:D:27:GLN:HG3	2.14	0.46
1:C:194:LEU:HB2	1:C:223:ILE:HD11	1.96	0.46
1:B:68:LEU:HD12	1:B:68:LEU:N	2.31	0.46
1:C:249:LEU:HA	1:C:310:THR:O	2.16	0.46
1:A:21:ASN:HA	3:A:332:HOH:O	2.15	0.46
1:B:94:SER:HB2	1:B:112:ASP:CG	2.36	0.46
1:A:95:VAL:O	1:A:99:VAL:HG23	2.15	0.46
1:C:207:GLN:HG2	1:D:52:THR:HB	1.98	0.46
1:A:149:LYS:HB3	1:B:201:ASN:ND2	2.31	0.46
1:D:79:ASP:HB2	1:D:138:THR:O	2.15	0.46
1:A:299:LEU:C	1:A:300:ILE:HG13	2.36	0.46
1:D:221:ARG:HD2	1:D:221:ARG:HA	1.76	0.46
1:D:188:GLY:O	1:D:191:TRP:HD1	1.99	0.46
1:D:21:ASN:HB3	1:D:50:ILE:O	2.16	0.46
1:B:253:SER:HB3	1:B:256:ILE:HG13	1.98	0.46
1:D:117:CYS:HB2	1:D:312:PHE:O	2.16	0.46
1:A:251:GLN:NE2	1:A:289:LEU:HD22	2.31	0.46
1:C:253:SER:HB3	1:C:256:ILE:HG13	1.97	0.46
1:B:117:CYS:HB2	1:B:312:PHE:O	2.15	0.46
1:C:310:THR:HG22	1:C:320:SER:HB3	1.96	0.46
1:A:194:LEU:HD13	1:A:218:MET:HB3	1.97	0.46
1:A:10:ARG:CD	1:A:174:ALA:HB2	2.35	0.45
1:C:264:THR:CG2	1:C:266:ILE:H	2.30	0.45
1:A:50:ILE:HG23	1:A:148:SER:CB	2.45	0.45
1:C:86:VAL:HG13	1:C:86:VAL:O	2.15	0.45
1:D:25:ASN:HB2	1:D:36:ASP:OD2	2.16	0.45
1:C:233:GLN:HA	1:C:233:GLN:NE2	2.31	0.45
1:B:80:PHE:HA	1:B:108:ALA:HB1	1.99	0.45
1:B:299:LEU:C	1:B:300:ILE:HG13	2.36	0.45
1:B:19:PRO:HD2	1:B:49:ARG:CB	2.46	0.45
1:B:306:ARG:HD2	3:B:333:HOH:O	2.17	0.45
1:B:323:LEU:C	1:B:323:LEU:HD12	2.37	0.45
1:A:147:PHE:CE2	1:A:282:SER:HB2	2.51	0.45
1:C:137:GLN:HE21	1:C:137:GLN:HB2	1.63	0.45
1:A:323:LEU:HD12	1:A:323:LEU:C	2.37	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:57:SER:HA	1:A:95:VAL:HG13	1.99	0.45
1:B:115:ALA:HB3	1:B:119:GLY:HA2	1.98	0.45
1:A:264:THR:HG23	1:A:266:ILE:H	1.82	0.45
1:B:146:THR:O	1:B:149:LYS:HG2	2.17	0.45
1:D:86:VAL:HG13	1:D:86:VAL:O	2.16	0.45
1:D:300:ILE:O	1:D:303:SER:OG	2.35	0.45
1:B:190:ARG:NH2	1:B:226:PHE:HB2	2.32	0.45
1:C:201:ASN:ND2	1:C:206:TYR:CD1	2.85	0.45
1:A:55:ASN:OD1	1:A:56:THR:N	2.41	0.45
1:C:195:THR:HG22	1:D:93:PRO:CD	2.41	0.44
1:D:252:ALA:HB1	2:D:401:ACO:H22	1.98	0.44
1:A:21:ASN:HB3	1:A:50:ILE:O	2.18	0.44
1:D:249:LEU:HA	1:D:310:THR:O	2.17	0.44
1:A:21:ASN:O	1:A:49:ARG:HA	2.17	0.44
1:C:57:SER:HA	1:C:95:VAL:HG13	1.99	0.44
1:C:90:PHE:HB3	1:D:196:SER:O	2.16	0.44
1:A:73:LYS:HE2	1:A:172:GLU:OE1	2.18	0.44
1:D:254:VAL:HA	1:D:275:MET:HE1	1.99	0.44
1:C:218:MET:SD	1:C:223:ILE:HD12	2.57	0.44
1:A:28:LEU:HB3	1:A:32:MET:CE	2.48	0.44
1:C:52:THR:C	1:C:53:GLN:HG3	2.37	0.44
1:B:303:SER:OG	1:B:305:GLN:CG	2.64	0.44
1:B:194:LEU:HD13	1:B:218:MET:HB3	1.98	0.44
1:C:50:ILE:HG23	1:C:148:SER:CB	2.48	0.44
1:A:14:THR:HG22	1:A:169:VAL:HG12	1.98	0.44
1:D:25:ASN:OD1	1:D:48:ARG:NH2	2.51	0.44
1:A:115:ALA:HB3	1:A:119:GLY:HA2	1.99	0.44
1:D:50:ILE:HG23	1:D:148:SER:CB	2.47	0.43
1:D:70:LYS:NZ	3:D:329:HOH:O	2.40	0.43
1:C:193:ALA:HA	1:C:219:GLU:HG3	2.00	0.43
1:A:8:TYR:CE2	1:A:177:PRO:HD3	2.53	0.43
1:C:241:ASP:HB2	1:C:266:ILE:HA	2.00	0.43
1:C:97:CYS:O	1:D:188:GLY:HA3	2.18	0.43
1:B:28:LEU:HB3	1:B:32:MET:CE	2.48	0.43
1:D:28:LEU:HB3	1:D:32:MET:CE	2.49	0.43
1:B:50:ILE:HG23	1:B:148:SER:CB	2.48	0.43
1:A:205:PHE:CD2	1:B:50:ILE:HG21	2.53	0.43
1:B:310:THR:HG22	1:B:320:SER:HB3	2.00	0.43
1:A:306:ARG:HH22	1:A:322:LEU:HD21	1.83	0.43
1:B:83:VAL:O	1:B:112:ASP:HA	2.17	0.43
1:B:57:SER:HA	1:B:95:VAL:HG13	1.99	0.43
1:C:147:PHE:CE2	1:C:282:SER:HB2	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:29:SER:HA	1:C:34:THR:HG23	2.00	0.43
1:A:68:LEU:HD12	1:A:68:LEU:N	2.32	0.43
1:C:83:VAL:O	1:C:112:ASP:HA	2.18	0.43
1:B:273:THR:CG2	1:B:274:ASN:N	2.81	0.43
1:B:48:ARG:O	1:B:49:ARG:HD3	2.19	0.43
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.64	0.43
1:A:100:GLN:NE2	1:A:108:ALA:O	2.48	0.43
1:B:64:ALA:O	1:B:68:LEU:HD13	2.18	0.43
1:C:155:ASP:OD2	1:C:157:SER:HB2	2.18	0.43
1:C:129:LYS:NZ	1:C:182:GLU:OE2	2.52	0.43
1:C:299:LEU:HA	1:C:305:GLN:HE22	1.84	0.43
1:A:86:VAL:N	1:A:145:GLU:OE2	2.45	0.43
1:A:147:PHE:HE2	1:A:282:SER:HB2	1.84	0.43
1:A:16:ARG:NH1	1:A:291:ASP:OD2	2.52	0.43
1:B:89:ASP:HB2	1:B:98:GLN:HE22	1.84	0.42
1:C:80:PHE:HA	1:C:108:ALA:HB1	2.01	0.42
1:B:129:LYS:NZ	1:B:182:GLU:OE2	2.52	0.42
1:C:191:TRP:CE3	1:D:93:PRO:HG3	2.55	0.42
1:B:261:ALA:C	1:B:264:THR:HG22	2.40	0.42
1:C:28:LEU:HB3	1:C:32:MET:CE	2.48	0.42
1:C:45:ILE:HA	1:C:276:ASP:HA	2.01	0.42
1:D:19:PRO:HD2	1:D:49:ARG:CB	2.50	0.42
1:D:80:PHE:HA	1:D:108:ALA:HB1	2.00	0.42
1:D:57:SER:HA	1:D:95:VAL:HG13	2.01	0.42
1:C:224:PHE:HB2	2:C:401:ACO:H143	2.02	0.42
1:D:310:THR:HG22	1:D:320:SER:HB3	2.00	0.42
1:A:38:TRP:CE2	1:A:42:ARG:HG3	2.55	0.42
1:D:48:ARG:HH11	1:D:48:ARG:CG	2.33	0.42
1:A:19:PRO:HD2	1:A:49:ARG:HB2	2.01	0.42
1:C:115:ALA:HB3	1:C:119:GLY:HA2	2.01	0.42
1:A:261:ALA:C	1:A:264:THR:HG22	2.40	0.42
1:D:299:LEU:HD23	1:D:305:GLN:HE21	1.84	0.42
1:A:310:THR:HG22	1:A:320:SER:HB3	2.01	0.42
1:C:48:ARG:HG2	3:C:4:HOH:O	2.19	0.41
1:C:261:ALA:C	1:C:264:THR:HG22	2.40	0.41
1:C:245:ASP:O	1:C:270:LYS:HG2	2.20	0.41
1:B:299:LEU:HA	1:B:305:GLN:NE2	2.34	0.41
1:D:251:GLN:OE1	1:D:274:ASN:N	2.52	0.41
1:C:308:VAL:HA	1:C:321:LEU:O	2.19	0.41
1:A:25:ASN:HB3	1:A:36:ASP:HA	2.01	0.41
1:A:300:ILE:H	1:A:305:GLN:NE2	2.15	0.41
1:B:147:PHE:CE2	1:B:282:SER:HB2	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:194:LEU:HD13	1:C:218:MET:HB3	2.02	0.41
1:D:167:ALA:HB3	1:D:287:PRO:HG2	2.02	0.41
1:D:115:ALA:HB3	1:D:119:GLY:HA2	2.01	0.41
1:C:300:ILE:H	1:C:305:GLN:NE2	2.18	0.41
1:D:6:LYS:HB2	1:D:175:GLU:OE2	2.20	0.41
1:D:8:TYR:CE2	1:D:177:PRO:HD3	2.55	0.41
1:D:147:PHE:CE2	1:D:282:SER:HB2	2.55	0.41
1:B:249:LEU:HG	1:B:310:THR:HG1	1.81	0.41
1:B:129:LYS:HZ1	1:B:182:GLU:CD	2.23	0.41
1:C:195:THR:HA	1:D:92:MET:O	2.20	0.41
1:B:178:HIS:HA	1:B:324:THR:HG23	2.01	0.41
1:B:86:VAL:HG13	1:B:86:VAL:O	2.20	0.41
1:D:19:PRO:HD2	1:D:49:ARG:HB3	2.01	0.41
1:D:147:PHE:HE2	1:D:282:SER:CB	2.33	0.41
1:B:308:VAL:HA	1:B:321:LEU:O	2.21	0.41
1:C:274:ASN:O	1:C:274:ASN:ND2	2.54	0.41
1:B:286:ILE:N	1:B:287:PRO:HD2	2.36	0.41
1:B:81:ILE:HB	1:B:110:ALA:HB2	2.03	0.41
1:A:188:GLY:HA3	1:B:97:CYS:O	2.19	0.41
1:A:274:ASN:ND2	1:A:292:GLU:OE2	2.42	0.41
1:A:286:ILE:N	1:A:287:PRO:HD2	2.35	0.41
1:B:268:ARG:O	1:B:268:ARG:HD2	2.20	0.41
1:A:117:CYS:HB2	1:A:312:PHE:O	2.20	0.41
1:C:255:ARG:NH1	2:C:401:ACO:OAP	2.54	0.41
1:A:310:THR:HG22	1:A:320:SER:OG	2.20	0.41
1:D:94:SER:HB2	1:D:112:ASP:CG	2.41	0.41
1:C:254:VAL:HA	1:C:275:MET:HE1	2.03	0.41
1:D:273:THR:HG21	3:D:331:HOH:O	2.20	0.41
1:A:147:PHE:HE2	1:A:282:SER:CB	2.34	0.41
1:A:6:LYS:HB2	1:A:175:GLU:OE2	2.20	0.40
1:A:74:GLN:HE21	1:A:74:GLN:HB3	1.56	0.40
1:A:50:ILE:HA	1:A:164:ASP:OD2	2.21	0.40
1:D:137:GLN:O	1:D:172:GLU:HA	2.22	0.40
1:C:147:PHE:HE2	1:C:282:SER:CB	2.34	0.40
1:A:254:VAL:HA	1:A:275:MET:HE1	2.03	0.40
1:C:7:ASN:O	1:C:131:VAL:HG12	2.20	0.40
1:B:226:PHE:CD2	1:B:316:LEU:HD23	2.57	0.40
1:B:33:ASP:OD1	1:B:33:ASP:C	2.60	0.40
1:D:129:LYS:N	1:D:129:LYS:HD2	2.35	0.40
1:D:221:ARG:NH1	2:D:401:ACO:H132	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	312/320 (98%)	286 (92%)	25 (8%)	1 (0%)	50 90
1	B	311/320 (97%)	284 (91%)	27 (9%)	0	100 100
1	C	311/320 (97%)	279 (90%)	31 (10%)	1 (0%)	50 90
1	D	312/320 (98%)	289 (93%)	21 (7%)	2 (1%)	33 81
All	All	1246/1280 (97%)	1138 (91%)	104 (8%)	4 (0%)	50 90

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	153	TRP
1	A	153	TRP
1	C	153	TRP
1	D	275	MET

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	266/267 (100%)	253 (95%)	13 (5%)	35 78
1	B	265/267 (99%)	249 (94%)	16 (6%)	27 69
1	C	265/267 (99%)	250 (94%)	15 (6%)	29 71
1	D	266/267 (100%)	252 (95%)	14 (5%)	32 74
All	All	1062/1068 (99%)	1004 (94%)	58 (6%)	30 73

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	49	ARG
1	A	54	GLU
1	A	74	GLN
1	A	86	VAL
1	A	137	GLN
1	A	145	GLU
1	A	170	LEU
1	A	180	LEU
1	A	199	THR
1	A	226	PHE
1	A	274	ASN
1	A	323	LEU
1	B	36	ASP
1	B	48	ARG
1	B	74	GLN
1	B	86	VAL
1	B	137	GLN
1	B	170	LEU
1	B	172	GLU
1	B	180	LEU
1	B	199	THR
1	B	226	PHE
1	B	264	THR
1	B	265	LYS
1	B	268	ARG
1	B	274	ASN
1	B	275	MET
1	B	323	LEU
1	C	48	ARG
1	C	86	VAL
1	C	137	GLN
1	C	170	LEU
1	C	180	LEU
1	C	199	THR
1	C	226	PHE
1	C	233	GLN
1	C	264	THR
1	C	268	ARG
1	C	269	GLU
1	C	274	ASN
1	C	275	MET
1	C	296	ASN

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Mol	Chain	Res	Type
1	C	323	LEU
1	D	10	ARG
1	D	47	GLU
1	D	48	ARG
1	D	65	LYS
1	D	86	VAL
1	D	137	GLN
1	D	170	LEU
1	D	180	LEU
1	D	199	THR
1	D	226	PHE
1	D	268	ARG
1	D	274	ASN
1	D	275	MET
1	D	323	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	74	GLN
1	A	91	ASN
1	A	98	GLN
1	A	137	GLN
1	A	189	GLN
1	A	207	GLN
1	A	233	GLN
1	A	304	GLN
1	A	305	GLN
1	B	25	ASN
1	B	27	GLN
1	B	53	GLN
1	B	91	ASN
1	B	98	GLN
1	B	137	GLN
1	B	189	GLN
1	B	274	ASN
1	B	280	ASN
1	B	304	GLN
1	B	305	GLN
1	C	7	ASN
1	C	25	ASN

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Mol	Chain	Res	Type
1	C	27	GLN
1	C	53	GLN
1	C	91	ASN
1	C	98	GLN
1	C	137	GLN
1	C	185	GLN
1	C	189	GLN
1	C	233	GLN
1	C	274	ASN
1	C	304	GLN
1	C	305	GLN
1	D	27	GLN
1	D	53	GLN
1	D	91	ASN
1	D	98	GLN
1	D	137	GLN
1	D	189	GLN
1	D	207	GLN
1	D	274	ASN
1	D	304	GLN
1	D	305	GLN

5.3.3 RNA

There are no RNA chains in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSO	A	13	1	6,6,7	6.92	3 (50%)	3,6,8	5.69	3 (100%)
1	CSO	A	22	1	6,6,7	7.54	3 (50%)	3,6,8	4.45	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CSO	B	13	1	6,6,7	6.93	3 (50%)	3,6,8	5.76	3 (100%)
1	CSO	B	22	1	6,6,7	7.42	3 (50%)	3,6,8	4.74	2 (66%)
1	CSO	C	13	1	6,6,7	7.16	4 (66%)	3,6,8	5.64	3 (100%)
1	CSO	C	22	1	6,6,7	7.24	3 (50%)	3,6,8	4.76	2 (66%)
1	CSO	D	13	1	6,6,7	7.08	3 (50%)	3,6,8	5.76	3 (100%)
1	CSO	D	22	1	6,6,7	7.63	3 (50%)	3,6,8	5.00	2 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	A	13	1	-	0/2/5/7	0/0/0/0
1	CSO	A	22	1	-	0/2/5/7	0/0/0/0
1	CSO	B	13	1	-	0/2/5/7	0/0/0/0
1	CSO	B	22	1	-	0/2/5/7	0/0/0/0
1	CSO	C	13	1	-	0/2/5/7	0/0/0/0
1	CSO	C	22	1	-	0/2/5/7	0/0/0/0
1	CSO	D	13	1	-	0/2/5/7	0/0/0/0
1	CSO	D	22	1	-	0/2/5/7	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	22	CSO	O-C	17.75	1.23	1.11
1	A	22	CSO	O-C	17.53	1.23	1.11
1	B	22	CSO	O-C	17.32	1.23	1.11
1	C	22	CSO	O-C	16.81	1.23	1.11
1	C	13	CSO	O-C	16.80	1.23	1.11
1	D	13	CSO	O-C	16.55	1.22	1.11
1	B	13	CSO	O-C	16.34	1.22	1.11
1	A	13	CSO	O-C	16.32	1.22	1.11
1	D	22	CSO	CA-C	4.40	1.56	1.48
1	A	22	CSO	CA-C	4.25	1.56	1.48
1	C	22	CSO	CA-C	4.14	1.56	1.48
1	B	22	CSO	CA-C	3.78	1.55	1.48
1	D	13	CSO	CA-C	3.71	1.55	1.48
1	B	22	CSO	CB-CA	3.59	1.60	1.52
1	C	22	CSO	CB-CA	3.50	1.59	1.52
1	D	22	CSO	CB-CA	3.34	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	CSO	CB-CA	3.22	1.59	1.52
1	A	13	CSO	CB-CA	3.18	1.59	1.52
1	C	13	CSO	CA-C	3.13	1.54	1.48
1	D	13	CSO	CB-CA	3.03	1.58	1.52
1	B	13	CSO	CA-C	2.92	1.53	1.48
1	B	13	CSO	CB-CA	2.80	1.58	1.52
1	C	13	CSO	CB-CA	2.66	1.58	1.52
1	A	13	CSO	CA-C	2.64	1.53	1.48
1	C	13	CSO	CB-SG	-2.29	1.79	1.82

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	13	CSO	C-CA-N	-8.09	105.75	113.83
1	D	13	CSO	C-CA-N	-7.87	105.97	113.83
1	A	13	CSO	C-CA-N	-7.86	105.98	113.83
1	C	13	CSO	C-CA-N	-7.69	106.15	113.83
1	D	22	CSO	C-CA-N	-7.45	106.39	113.83
1	C	22	CSO	C-CA-N	-7.30	106.54	113.83
1	B	22	CSO	C-CA-N	-7.24	106.59	113.83
1	A	22	CSO	C-CA-N	-6.77	107.06	113.83
1	A	13	CSO	CB-CA-N	5.14	118.99	110.27
1	D	13	CSO	CB-CA-N	5.04	118.82	110.27
1	B	13	CSO	CB-CA-N	4.72	118.27	110.27
1	C	13	CSO	CB-CA-N	4.57	118.03	110.27
1	D	22	CSO	CB-CA-N	4.03	117.10	110.27
1	C	13	CSO	CA-CB-SG	-3.94	106.01	113.01
1	B	22	CSO	CB-CA-N	3.50	116.21	110.27
1	C	22	CSO	CB-CA-N	3.49	116.19	110.27
1	D	13	CSO	CA-CB-SG	-3.49	106.81	113.01
1	B	13	CSO	CA-CB-SG	-3.45	106.87	113.01
1	A	22	CSO	CB-CA-N	3.22	115.73	110.27
1	A	13	CSO	CA-CB-SG	-3.02	107.64	113.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACO	A	401	-	53,53,53	2.57	20 (37%)	79,79,79	2.51	24 (30%)
2	ACO	B	401	-	53,53,53	2.81	20 (37%)	79,79,79	2.52	22 (27%)
2	ACO	C	401	-	53,53,53	2.67	24 (45%)	79,79,79	2.54	28 (35%)
2	ACO	D	401	-	53,53,53	2.69	20 (37%)	79,79,79	2.57	28 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACO	A	401	-	-	2/51/67/67	0/1/3/3
2	ACO	B	401	-	-	3/51/67/67	0/1/3/3
2	ACO	C	401	-	-	2/51/67/67	0/1/3/3
2	ACO	D	401	-	-	2/51/67/67	0/1/3/3

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ACO	CBP-CAP	10.54	1.66	1.55
2	C	401	ACO	CBP-CAP	10.49	1.66	1.55
2	B	401	ACO	CBP-CAP	10.14	1.66	1.55
2	A	401	ACO	CBP-CAP	10.09	1.66	1.55
2	B	401	ACO	P1A-O3A	5.52	1.69	1.59
2	C	401	ACO	C4A-N9A	-5.29	1.30	1.37
2	A	401	ACO	C4A-N9A	-5.21	1.30	1.37
2	D	401	ACO	C4A-N9A	-5.17	1.30	1.37
2	C	401	ACO	C-S1P	-5.17	1.52	1.75
2	B	401	ACO	C-S1P	-5.03	1.53	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ACO	P2A-O3A	4.90	1.68	1.59
2	C	401	ACO	C2A-N3A	4.88	1.41	1.32
2	B	401	ACO	C4A-N9A	-4.87	1.30	1.37
2	B	401	ACO	C2A-N3A	4.81	1.41	1.32
2	D	401	ACO	C2A-N3A	4.76	1.41	1.32
2	A	401	ACO	C2A-N3A	4.54	1.41	1.32
2	B	401	ACO	O4B-C1B	4.50	1.48	1.41
2	D	401	ACO	C-S1P	-4.35	1.56	1.75
2	A	401	ACO	CH3-C	4.33	1.66	1.50
2	C	401	ACO	O4B-C1B	4.31	1.48	1.41
2	A	401	ACO	C-S1P	-4.19	1.57	1.75
2	D	401	ACO	O4B-C1B	4.12	1.47	1.41
2	C	401	ACO	CH3-C	4.07	1.65	1.50
2	B	401	ACO	CH3-C	4.03	1.65	1.50
2	D	401	ACO	CH3-C	4.02	1.65	1.50
2	C	401	ACO	C2B-C1B	3.93	1.59	1.53
2	D	401	ACO	C8A-N9A	3.80	1.42	1.36
2	B	401	ACO	C4A-N3A	3.74	1.41	1.35
2	B	401	ACO	C8A-N9A	3.68	1.42	1.36
2	D	401	ACO	P1A-O3A	3.56	1.66	1.59
2	B	401	ACO	CCP-CBP	3.52	1.58	1.52
2	D	401	ACO	CCP-CBP	3.48	1.58	1.52
2	B	401	ACO	C8A-N7A	3.47	1.41	1.34
2	A	401	ACO	C8A-N9A	3.45	1.41	1.36
2	D	401	ACO	C4A-N3A	3.44	1.40	1.35
2	A	401	ACO	C2B-C1B	3.44	1.58	1.53
2	D	401	ACO	C8A-N7A	3.41	1.41	1.34
2	C	401	ACO	C8A-N7A	3.36	1.41	1.34
2	A	401	ACO	C8A-N7A	3.31	1.41	1.34
2	B	401	ACO	C2B-C1B	3.31	1.58	1.53
2	C	401	ACO	C4A-N3A	3.30	1.40	1.35
2	D	401	ACO	C2B-C1B	3.29	1.58	1.53
2	A	401	ACO	P1A-O3A	3.26	1.65	1.59
2	C	401	ACO	C8A-N9A	3.25	1.41	1.36
2	D	401	ACO	O-C	3.15	1.33	1.21
2	A	401	ACO	P3B-O7A	3.13	1.61	1.51
2	D	401	ACO	P2A-O3A	3.08	1.65	1.59
2	A	401	ACO	O-C	3.07	1.32	1.21
2	D	401	ACO	P3B-O7A	3.05	1.61	1.51
2	A	401	ACO	C4A-N3A	3.03	1.40	1.35
2	A	401	ACO	O4B-C1B	3.02	1.46	1.41
2	B	401	ACO	P3B-O7A	2.90	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	ACO	CCP-CBP	2.80	1.57	1.52
2	B	401	ACO	O-C	2.75	1.31	1.21
2	C	401	ACO	C9P-N8P	2.75	1.39	1.33
2	C	401	ACO	O-C	2.73	1.31	1.21
2	A	401	ACO	C9P-N8P	2.69	1.39	1.33
2	B	401	ACO	P3B-O3B	2.65	1.68	1.59
2	A	401	ACO	CCP-CBP	2.60	1.56	1.52
2	C	401	ACO	P3B-O7A	2.59	1.59	1.51
2	C	401	ACO	C5A-N7A	-2.58	1.30	1.40
2	D	401	ACO	C9P-N8P	2.56	1.39	1.33
2	B	401	ACO	C9P-N8P	2.56	1.39	1.33
2	A	401	ACO	C5A-N7A	-2.46	1.31	1.40
2	C	401	ACO	P1A-O3A	2.45	1.64	1.59
2	A	401	ACO	P3B-O8A	2.41	1.63	1.54
2	C	401	ACO	O9P-C9P	2.36	1.28	1.23
2	B	401	ACO	C5A-N7A	-2.34	1.31	1.40
2	A	401	ACO	O9P-C9P	2.32	1.28	1.23
2	A	401	ACO	P3B-O3B	2.32	1.67	1.59
2	D	401	ACO	C5A-N7A	-2.30	1.31	1.40
2	D	401	ACO	C5A-C4A	2.27	1.45	1.40
2	B	401	ACO	O9P-C9P	2.20	1.27	1.23
2	C	401	ACO	P1A-O1A	2.19	1.59	1.51
2	C	401	ACO	P3B-O8A	2.14	1.62	1.54
2	C	401	ACO	C2B-C3B	-2.13	1.48	1.53
2	C	401	ACO	P3B-O3B	2.10	1.66	1.59
2	B	401	ACO	C5A-C4A	2.09	1.45	1.40
2	C	401	ACO	O5P-C5P	2.08	1.27	1.23
2	D	401	ACO	P3B-O8A	2.06	1.62	1.54
2	D	401	ACO	P3B-O3B	2.05	1.66	1.59
2	C	401	ACO	C5A-C4A	2.05	1.45	1.40
2	A	401	ACO	C5A-C4A	2.02	1.45	1.40
2	C	401	ACO	P1A-O5B	2.02	1.68	1.59

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	ACO	N3A-C2A-N1A	-10.44	119.98	128.71
2	C	401	ACO	N3A-C2A-N1A	-10.18	120.20	128.71
2	A	401	ACO	N3A-C2A-N1A	-10.11	120.26	128.71
2	D	401	ACO	N3A-C2A-N1A	-10.09	120.27	128.71
2	D	401	ACO	O-C-CH3	-6.91	99.49	123.20
2	A	401	ACO	O-C-CH3	-6.80	99.87	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	ACO	O-C-CH3	-6.68	100.28	123.20
2	B	401	ACO	O-C-CH3	-6.56	100.69	123.20
2	A	401	ACO	C1B-N9A-C4A	-6.23	115.87	126.64
2	D	401	ACO	C1B-N9A-C4A	-6.16	115.99	126.64
2	D	401	ACO	CBP-CAP-C9P	6.16	118.71	112.73
2	B	401	ACO	C1B-N9A-C4A	-6.15	116.02	126.64
2	C	401	ACO	CBP-CAP-C9P	6.01	118.56	112.73
2	C	401	ACO	C1B-N9A-C4A	-5.90	116.44	126.64
2	B	401	ACO	CBP-CAP-C9P	5.87	118.42	112.73
2	A	401	ACO	C8A-N9A-C4A	5.34	110.98	106.90
2	C	401	ACO	C8A-N9A-C4A	5.28	110.93	106.90
2	B	401	ACO	C8A-N9A-C4A	5.23	110.89	106.90
2	D	401	ACO	C8A-N9A-C4A	5.23	110.89	106.90
2	C	401	ACO	C3P-N4P-C5P	4.81	132.63	122.84
2	A	401	ACO	CBP-CAP-C9P	4.81	117.39	112.73
2	D	401	ACO	O4B-C1B-C2B	-4.78	99.44	106.77
2	D	401	ACO	C3P-N4P-C5P	4.48	131.95	122.84
2	A	401	ACO	C3P-N4P-C5P	4.41	131.81	122.84
2	A	401	ACO	O4B-C1B-C2B	-4.37	100.07	106.77
2	D	401	ACO	C7P-N8P-C9P	4.17	131.14	122.57
2	B	401	ACO	C3P-N4P-C5P	4.16	131.30	122.84
2	A	401	ACO	C7P-N8P-C9P	4.08	130.96	122.57
2	C	401	ACO	N3A-C4A-N9A	4.03	132.71	125.43
2	B	401	ACO	C7P-N8P-C9P	4.00	130.80	122.57
2	A	401	ACO	C2P-C3P-N4P	-3.95	103.56	112.50
2	D	401	ACO	N3A-C4A-N9A	3.94	132.55	125.43
2	B	401	ACO	N3A-C4A-N9A	3.90	132.48	125.43
2	B	401	ACO	O5P-C5P-N4P	-3.83	115.34	122.94
2	A	401	ACO	N3A-C4A-N9A	3.81	132.31	125.43
2	A	401	ACO	CH3-C-S1P	3.71	130.12	113.71
2	C	401	ACO	C7P-N8P-C9P	3.71	130.20	122.57
2	C	401	ACO	O4B-C1B-C2B	-3.66	101.17	106.77
2	A	401	ACO	O5P-C5P-N4P	-3.65	115.69	122.94
2	D	401	ACO	CH3-C-S1P	3.55	129.41	113.71
2	B	401	ACO	O4B-C1B-C2B	-3.53	101.36	106.77
2	A	401	ACO	CDP-CBP-CAP	3.50	114.89	108.82
2	D	401	ACO	CCP-CBP-CAP	3.50	113.81	108.70
2	B	401	ACO	CCP-CBP-CAP	3.47	113.77	108.70
2	A	401	ACO	C8A-N9A-C1B	3.44	133.15	126.38
2	D	401	ACO	C8A-N9A-C1B	3.42	133.12	126.38
2	B	401	ACO	C8A-N9A-C1B	3.40	133.09	126.38
2	C	401	ACO	CH3-C-S1P	3.37	128.60	113.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	ACO	N7A-C8A-N9A	-3.35	104.88	114.36
2	B	401	ACO	CH3-C-S1P	3.33	128.44	113.71
2	C	401	ACO	N7A-C8A-N9A	-3.32	104.96	114.36
2	C	401	ACO	CDP-CBP-CCP	-3.31	103.99	108.76
2	B	401	ACO	N7A-C8A-N9A	-3.30	105.02	114.36
2	B	401	ACO	C2P-C3P-N4P	-3.28	105.09	112.50
2	D	401	ACO	O5P-C5P-N4P	-3.26	116.47	122.94
2	D	401	ACO	C2P-C3P-N4P	-3.26	105.13	112.50
2	D	401	ACO	N7A-C8A-N9A	-3.25	105.17	114.36
2	C	401	ACO	O5P-C5P-N4P	-3.24	116.52	122.94
2	C	401	ACO	C8A-N9A-C1B	3.17	132.63	126.38
2	C	401	ACO	CDP-CBP-CAP	3.16	114.30	108.82
2	C	401	ACO	C2P-C3P-N4P	-3.16	105.35	112.50
2	D	401	ACO	CDP-CBP-CAP	3.03	114.08	108.82
2	D	401	ACO	C4B-O4B-C1B	3.01	113.02	109.75
2	C	401	ACO	CCP-CBP-CAP	3.00	113.09	108.70
2	C	401	ACO	O2B-C2B-C3B	3.00	120.01	111.20
2	D	401	ACO	O2B-C2B-C3B	2.99	119.99	111.20
2	B	401	ACO	C4B-O4B-C1B	2.97	112.97	109.75
2	B	401	ACO	CDP-CBP-CAP	2.91	113.87	108.82
2	A	401	ACO	C2A-N1A-C6A	2.85	123.92	118.77
2	B	401	ACO	O2B-C2B-C3B	2.85	119.58	111.20
2	B	401	ACO	C2A-N1A-C6A	2.84	123.89	118.77
2	D	401	ACO	C2A-N1A-C6A	2.83	123.88	118.77
2	A	401	ACO	O2B-C2B-C3B	2.71	119.17	111.20
2	C	401	ACO	C2A-N1A-C6A	2.69	123.62	118.77
2	C	401	ACO	N6A-C6A-N1A	2.68	124.63	119.36
2	B	401	ACO	N6A-C6A-N1A	2.63	124.52	119.36
2	A	401	ACO	N6A-C6A-N1A	2.59	124.45	119.36
2	D	401	ACO	N6A-C6A-N1A	2.54	124.35	119.36
2	A	401	ACO	C6P-C5P-N4P	2.53	121.10	116.50
2	D	401	ACO	C6P-C5P-N4P	2.43	120.91	116.50
2	D	401	ACO	CEP-CBP-CCP	-2.33	105.40	108.76
2	C	401	ACO	P2A-O3A-P1A	-2.32	124.88	131.68
2	A	401	ACO	C4B-O4B-C1B	2.31	112.26	109.75
2	C	401	ACO	C4B-O4B-C1B	2.29	112.23	109.75
2	B	401	ACO	C6P-C5P-N4P	2.22	120.53	116.50
2	C	401	ACO	CEP-CBP-CCP	-2.21	105.57	108.76
2	A	401	ACO	O-C-S1P	2.19	129.93	122.06
2	B	401	ACO	CDP-CBP-CCP	-2.18	105.62	108.76
2	C	401	ACO	O8A-P3B-O3B	-2.17	100.83	107.09
2	D	401	ACO	C6P-C7P-N8P	2.17	116.55	111.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	ACO	O9A-P3B-O8A	2.16	116.03	107.61
2	D	401	ACO	CDP-CBP-CCP	-2.14	105.67	108.76
2	A	401	ACO	C7P-C6P-C5P	-2.11	108.65	112.25
2	D	401	ACO	O8A-P3B-O3B	-2.11	101.03	107.09
2	C	401	ACO	C5A-C4A-N3A	-2.10	121.14	125.70
2	C	401	ACO	O4B-C4B-C3B	-2.08	100.15	104.88
2	D	401	ACO	O-C-S1P	2.07	129.52	122.06
2	D	401	ACO	C5A-C4A-N3A	-2.05	121.23	125.70
2	C	401	ACO	O2B-C2B-C1B	2.03	117.37	111.23
2	D	401	ACO	O9A-P3B-O8A	2.02	115.46	107.61
2	A	401	ACO	O9A-P3B-O8A	2.01	115.45	107.61
2	A	401	ACO	CDP-CBP-CCP	-2.01	105.86	108.76

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	ACO	O-C-S1P-C2P
2	C	401	ACO	O-C-S1P-C2P
2	A	401	ACO	CH3-C-S1P-C2P
2	B	401	ACO	O-C-S1P-C2P
2	D	401	ACO	CH3-C-S1P-C2P
2	A	401	ACO	O-C-S1P-C2P
2	C	401	ACO	CH3-C-S1P-C2P
2	B	401	ACO	CH3-C-S1P-C2P
2	B	401	ACO	C2B-C1B-N9A-C8A

There are no ring outliers.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	318/320 (99%)	-0.46	0	100	100	2, 23, 50, 103	0
1	B	317/320 (99%)	-0.43	0	100	100	3, 25, 54, 95	0
1	C	317/320 (99%)	-0.42	0	100	100	3, 27, 58, 99	0
1	D	318/320 (99%)	-0.42	0	100	100	4, 25, 51, 83	0
All	All	1270/1280 (99%)	-0.43	0	100	100	2, 25, 53, 103	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CSO	D	22	7/8	0.17	0.12	22,22,33,33	0
1	CSO	C	13	7/8	0.13	-0.46	36,36,43,43	0
1	CSO	A	22	7/8	0.14	-0.65	20,20,26,26	0
1	CSO	A	13	7/8	0.12	-0.66	29,29,37,37	0
1	CSO	B	22	7/8	0.13	-0.80	16,16,29,29	0
1	CSO	D	13	7/8	0.10	-1.16	7,7,16,16	0
1	CSO	B	13	7/8	0.10	-1.22	27,27,36,36	0
1	CSO	C	22	7/8	0.12	-1.63	16,16,26,26	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ACO	B	401	51/51	0.36	6.25	91,91,91,91	0
2	ACO	D	401	51/51	0.26	1.48	66,66,66,66	0
2	ACO	C	401	51/51	0.19	0.62	47,47,47,47	0
2	ACO	A	401	51/51	0.18	0.47	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.