Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:25 PM GMT

PDB ID	:	5CVU
Title	:	sinpyl alcohol bound monolignol 4-O-methyltransferase 5
Authors	:	Cai, Y.; Liu, C.-J.
Deposited on	:	2015-07-27
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

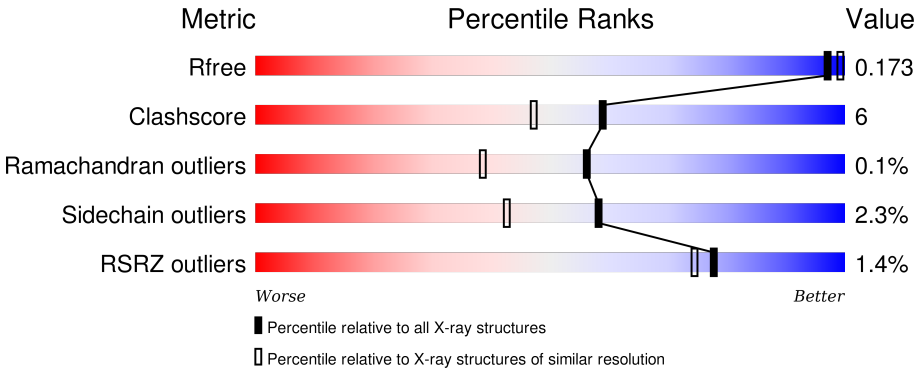
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	368	85% 10%
1	B	368	85% 12%
1	C	368	82% 13%
1	D	368	86% 11%

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	55B	A	401	-	X	-	X
2	55B	B	401	-	-	-	X
2	55B	C	401	-	-	-	X
2	55B	D	401	-	-	-	X
4	NO3	A	404	-	-	-	X
4	NO3	A	405	-	-	-	X
4	NO3	B	403	-	-	-	X
4	NO3	C	403	-	-	-	X
4	NO3	D	403	-	-	-	X
4	NO3	D	404	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11634 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.

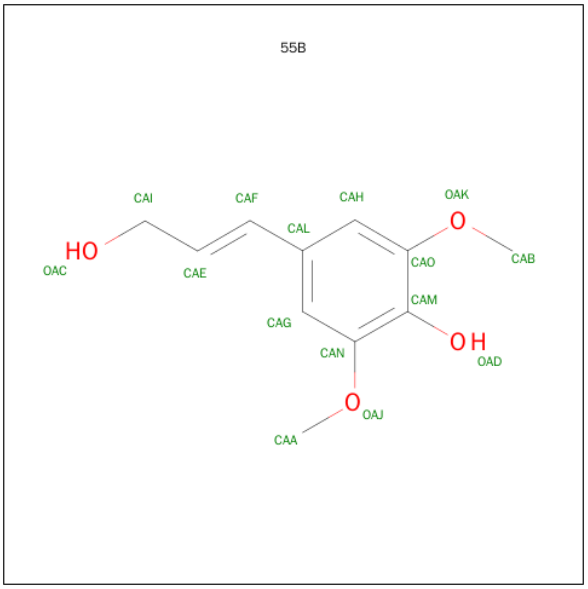
- Molecule 1 is a protein called (Iso)eugenol O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2714	1758	436	502	18			
1	B	360	Total	C	N	O	S	0	0	0
			2761	1790	443	510	18			
1	C	354	Total	C	N	O	S	0	0	0
			2714	1758	436	502	18			
1	D	361	Total	C	N	O	S	0	0	0
			2770	1795	444	513	18			

There are 20 discrepancies between the modelled and reference sequences:

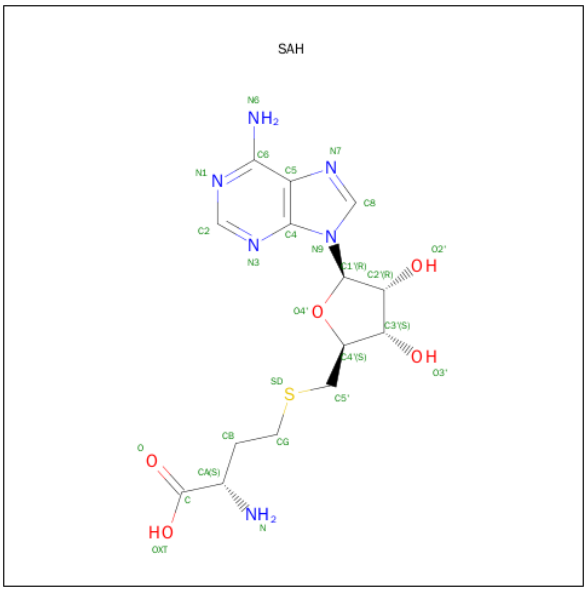
Chain	Residue	Modelled	Actual	Comment	Reference
A	133	LEU	THR	engineered mutation	UNP O04385
A	165	ILE	GLU	engineered mutation	UNP O04385
A	166	TRP	PHE	engineered mutation	UNP O04385
A	169	PHE	HIS	engineered mutation	UNP O04385
A	175	ILE	PHE	engineered mutation	UNP O04385
B	133	LEU	THR	engineered mutation	UNP O04385
B	165	ILE	GLU	engineered mutation	UNP O04385
B	166	TRP	PHE	engineered mutation	UNP O04385
B	169	PHE	HIS	engineered mutation	UNP O04385
B	175	ILE	PHE	engineered mutation	UNP O04385
C	133	LEU	THR	engineered mutation	UNP O04385
C	165	ILE	GLU	engineered mutation	UNP O04385
C	166	TRP	PHE	engineered mutation	UNP O04385
C	169	PHE	HIS	engineered mutation	UNP O04385
C	175	ILE	PHE	engineered mutation	UNP O04385
D	133	LEU	THR	engineered mutation	UNP O04385
D	165	ILE	GLU	engineered mutation	UNP O04385
D	166	TRP	PHE	engineered mutation	UNP O04385
D	169	PHE	HIS	engineered mutation	UNP O04385
D	175	ILE	PHE	engineered mutation	UNP O04385

- Molecule 2 is 4-[(1E)-3-hydroxyprop-1-en-1-yl]-2,6-dimethoxyphenol (three-letter code: 55B) (formula: $C_{11}H_{14}O_4$).



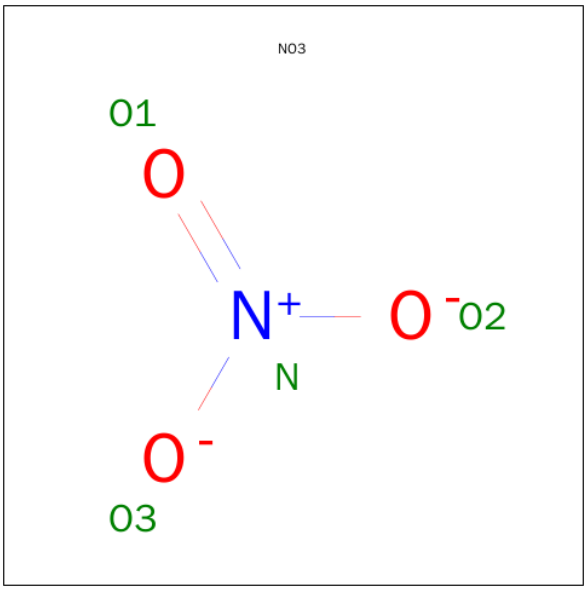
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 15 11 4	0	0
2	B	1	Total C O 15 11 4	0	0
2	C	1	Total C O 15 11 4	0	0
2	D	1	Total C O 15 11 4	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N O 4 1 3	0	0
4	A	1	Total N O 4 1 3	0	0
4	A	1	Total N O 4 1 3	0	0
4	B	1	Total N O 4 1 3	0	0
4	C	1	Total N O 4 1 3	0	0
4	C	1	Total N O 4 1 3	0	0
4	C	1	Total N O 4 1 3	0	0
4	D	1	Total N O 4 1 3	0	0
4	D	1	Total N O 4 1 3	0	0

- Molecule 5 is water.

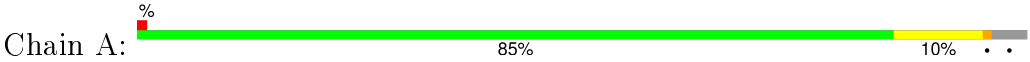
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	142	Total O 142 142	0	0
5	B	103	Total O 103 103	0	0
5	C	128	Total O 128 128	0	0
5	D	102	Total O 102 102	0	0

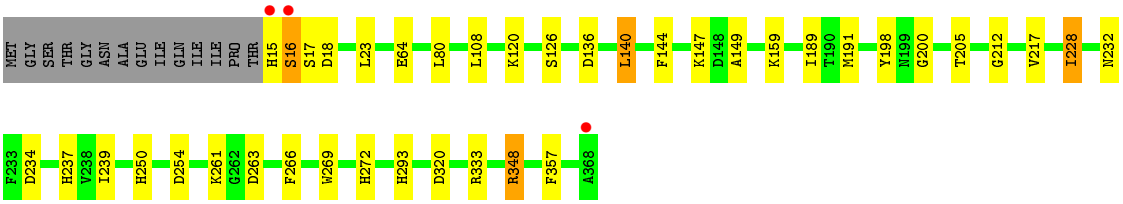
3 Residue-property plots (i)

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

- Molecule 1: (Iso)eugenol O-methyltransferase

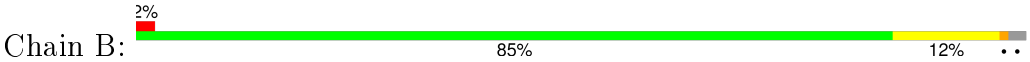
Chain A:

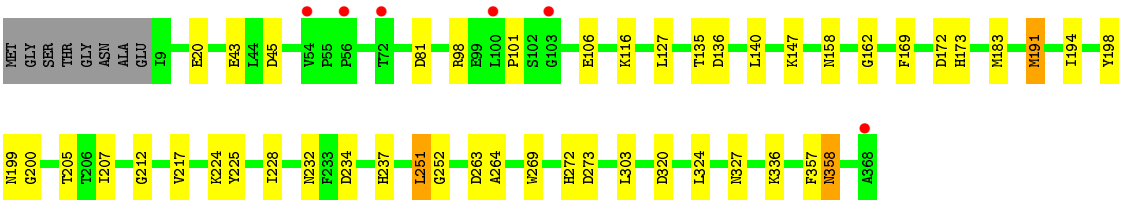




- Molecule 1: (Iso)eugenol O-methyltransferase

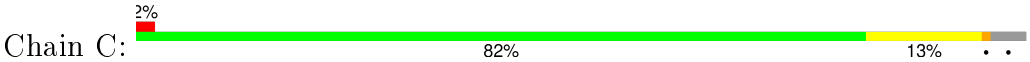
Chain B:

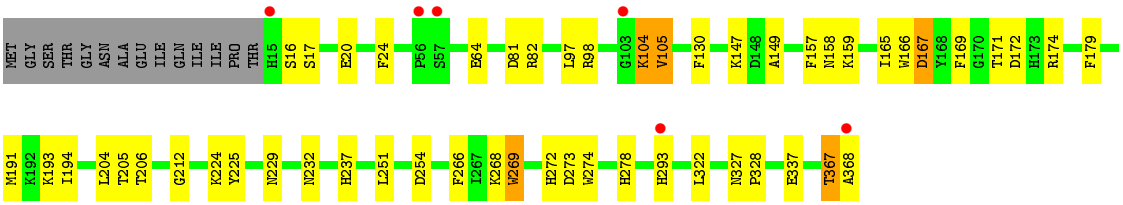




- Molecule 1: (Iso)eugenol O-methyltransferase

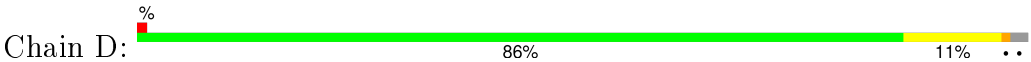
Chain C:

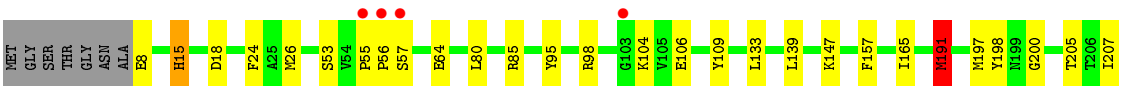




- Molecule 1: (Iso)eugenol O-methyltransferase

Chain D:






N229
P236
H237
Q240
L251
D254
K261
W269
H272
E277
L283
S306
R333
R348
F357
N358
A368

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.54Å 151.63Å 68.39Å 90.00° 92.55° 90.00°	Depositor
Resolution (Å)	75.81 – 1.80 50.75 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.9 (75.81-1.80) 88.6 (50.75-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.168 , 0.168 0.173 , 0.173	Depositor DCC
R_{free} test set	5957 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	15.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.4	EDS
Estimated twinning fraction	0.004 for l,k,-h 0.025 for h,-k,-l 0.019 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 156818 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11634	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, NO3, 55B

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	1.17	3/2781 (0.1%)	1.21	11/3779 (0.3%)
1	B	1.10	2/2829 (0.1%)	1.14	10/3846 (0.3%)
1	C	1.11	1/2781 (0.0%)	1.19	17/3779 (0.4%)
1	D	1.10	7/2838 (0.2%)	1.17	13/3858 (0.3%)
All	All	1.12	13/11229 (0.1%)	1.18	51/15262 (0.3%)

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

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	GLU	CD-OE2	7.45	1.33	1.25
1	C	64	GLU	CD-OE1	6.64	1.32	1.25
1	A	64	GLU	CG-CD	6.13	1.61	1.51
1	D	53	SER	CB-OG	-6.05	1.34	1.42
1	D	109	TYR	CE1-CZ	5.53	1.45	1.38
1	D	333	ARG	CZ-NH1	5.39	1.40	1.33
1	D	64	GLU	CG-CD	5.30	1.59	1.51
1	D	64	GLU	CD-OE1	5.21	1.31	1.25
1	D	95	TYR	CE1-CZ	5.16	1.45	1.38
1	B	20	GLU	CD-OE2	5.15	1.31	1.25
1	A	357	PHE	CE2-CZ	5.10	1.47	1.37
1	D	85	ARG	CZ-NH1	5.08	1.39	1.33
1	B	162	GLY	N-CA	5.08	1.53	1.46

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	191	MET	CG-SD-CE	-10.28	83.75	100.20
1	C	81	ASP	CB-CG-OD1	9.20	126.58	118.30
1	A	228	ILE	CG1-CB-CG2	-8.65	92.38	111.40
1	A	261	LYS	CD-CE-NZ	-8.17	92.91	111.70
1	D	348	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	C	169	PHE	CB-CG-CD2	-7.49	115.56	120.80
1	A	108	LEU	CB-CG-CD2	-7.26	98.66	111.00
1	D	147	LYS	CD-CE-NZ	-7.01	95.58	111.70
1	C	254	ASP	CB-CG-OD1	6.81	124.43	118.30
1	B	183	MET	CG-SD-CE	-6.68	89.51	100.20
1	D	191	MET	CG-SD-CE	6.56	110.69	100.20
1	D	18	ASP	CB-CG-OD1	6.54	124.18	118.30
1	D	18	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	C	98	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	320	ASP	CB-CG-OD2	6.47	124.12	118.30
1	D	254	ASP	CB-CG-OD1	6.42	124.08	118.30
1	C	24	PHE	CB-CG-CD1	6.41	125.29	120.80
1	A	333	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	D	333	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	303	LEU	CB-CG-CD1	-6.03	100.74	111.00
1	A	254	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	234	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	81	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	174	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	D	133	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	B	320	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	D	348	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	172	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	98	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	C	251	LEU	CB-CG-CD2	-5.54	101.58	111.00
1	C	24	PHE	CB-CG-CD2	-5.50	116.95	120.80
1	C	179	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	A	348	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	204	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	C	251	LEU	CA-CB-CG	5.34	127.57	115.30
1	C	167	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	80	LEU	CB-CG-CD1	-5.30	101.99	111.00
1	B	251	LEU	CA-CB-CG	5.29	127.48	115.30
1	C	82	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	A	120	LYS	CD-CE-NZ	-5.20	99.75	111.70
1	C	273	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	64	GLU	OE1-CD-OE2	-5.14	117.13	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	169	PHE	CB-CG-CD1	5.14	124.40	120.80
1	D	80	LEU	CB-CG-CD1	-5.14	102.27	111.00
1	D	24	PHE	CB-CG-CD2	-5.11	117.23	120.80
1	C	172	ASP	CB-CG-OD1	5.06	122.86	118.30
1	B	324	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	B	169	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	A	136	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	B	127	LEU	CB-CG-CD2	-5.01	102.48	111.00
1	D	24	PHE	CB-CG-CD1	5.01	124.31	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	367	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2714	0	2726	37	0
1	B	2761	0	2781	32	0
1	C	2714	0	2726	39	0
1	D	2770	0	2787	27	0
2	A	15	0	14	3	0
2	B	15	0	14	4	0
2	C	15	0	14	4	0
2	D	15	0	14	5	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
3	C	26	0	19	1	0
3	D	26	0	19	0	0
4	A	12	0	0	0	0
4	B	4	0	0	0	0
4	C	12	0	0	0	0
4	D	8	0	0	0	0
5	A	142	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	103	0	0	2	0
5	C	128	0	0	2	0
5	D	102	0	0	4	0
All	All	11634	0	11152	129	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 6.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:MET:HE2	1:B:194:ILE:HD12	1.15	1.09
1:C:193:LYS:HZ1	1:D:15:HIS:CD2	1.74	1.05
1:B:191:MET:CE	1:B:194:ILE:HD12	1.90	1.01
1:B:191:MET:HE2	1:B:194:ILE:CD1	1.91	0.99
1:C:191:MET:HE1	1:C:194:ILE:HD12	1.45	0.95
1:A:191:MET:HE1	1:A:266:PHE:CZ	2.00	0.95
1:A:191:MET:HE3	1:A:217:VAL:CG1	1.99	0.92
1:C:193:LYS:NZ	1:D:15:HIS:CD2	2.39	0.91
1:D:98:ARG:CD	1:D:106:GLU:OE1	2.19	0.90
1:B:98:ARG:HD2	1:B:106:GLU:OE1	1.74	0.88
1:A:191:MET:CE	1:A:217:VAL:CG1	2.54	0.86
1:A:140:LEU:HD23	1:A:140:LEU:O	1.78	0.84
1:D:98:ARG:HD3	1:D:106:GLU:OE1	1.79	0.82
1:A:191:MET:CE	1:A:217:VAL:HG11	2.09	0.81
1:A:140:LEU:HD23	1:A:140:LEU:C	2.01	0.80
1:D:98:ARG:HD2	1:D:106:GLU:OE1	1.80	0.79
1:A:191:MET:HE3	1:A:217:VAL:HG13	1.62	0.79
1:B:191:MET:CE	1:B:194:ILE:CD1	2.59	0.77
1:C:104:LYS:HD3	1:C:104:LYS:H	1.50	0.76
1:A:293:HIS:H	1:A:293:HIS:CD2	2.00	0.76
1:C:191:MET:HE1	1:C:194:ILE:CD1	2.14	0.75
1:A:191:MET:CE	1:A:217:VAL:HG13	2.17	0.74
1:A:191:MET:CE	1:A:266:PHE:CZ	2.72	0.73
1:B:357:PHE:O	1:B:358:ASN:HB2	1.88	0.73
1:C:191:MET:CE	1:C:194:ILE:HD12	2.19	0.71
1:A:191:MET:HE2	1:A:217:VAL:HG11	1.72	0.69
1:B:191:MET:HG3	1:B:217:VAL:HG22	1.74	0.68
1:B:136:ASP:O	1:B:140:LEU:HD13	1.94	0.68
1:C:269:TRP:CH2	2:C:401:55B:H1	2.30	0.66
1:C:193:LYS:NZ	1:D:15:HIS:HD2	1.91	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:C	1:A:140:LEU:CD2	2.65	0.64
1:D:277:GLU:HG2	5:D:503:HOH:O	1.96	0.64
1:A:191:MET:HE2	1:A:217:VAL:CG1	2.28	0.63
1:C:328:PRO:HD2	5:C:569:HOH:O	1.99	0.62
1:C:104:LYS:HD3	1:C:104:LYS:N	2.13	0.62
1:B:98:ARG:CD	1:B:106:GLU:OE1	2.46	0.62
1:B:357:PHE:O	1:B:358:ASN:CB	2.49	0.60
1:A:15:HIS:HB3	1:A:17:SER:HB3	1.83	0.60
1:C:130:PHE:CE2	1:D:26:MET:HE1	2.36	0.60
1:A:191:MET:HE3	1:A:217:VAL:HG11	1.76	0.59
1:A:147:LYS:HD3	1:B:43:GLU:HB3	1.87	0.57
1:A:140:LEU:HD21	1:A:144:PHE:CE2	2.39	0.56
1:A:15:HIS:CG	1:A:16:SER:H	2.24	0.56
1:C:167:ASP:O	1:C:171:THR:HG23	2.06	0.56
1:D:55:PRO:HB2	1:D:56:PRO:HD2	1.88	0.55
1:C:16:SER:O	1:C:20:GLU:HG2	2.06	0.55
1:A:140:LEU:CD2	1:A:144:PHE:CE2	2.90	0.55
1:D:269:TRP:CZ2	2:D:401:55B:H1	2.42	0.55
1:A:140:LEU:HD21	1:A:144:PHE:CZ	2.43	0.54
1:D:55:PRO:HG2	1:D:57:SER:HB2	1.90	0.54
1:C:17:SER:HA	1:C:20:GLU:OE1	2.08	0.54
1:A:15:HIS:CG	1:A:16:SER:N	2.76	0.53
1:A:237:HIS:HE1	5:A:600:HOH:O	1.91	0.53
1:C:237:HIS:HE1	5:C:601:HOH:O	1.91	0.53
1:A:191:MET:HG3	1:A:217:VAL:HG22	1.90	0.53
1:A:269:TRP:CZ2	2:A:401:55B:H6	2.43	0.53
1:B:212:GLY:HA3	1:B:232:ASN:ND2	2.24	0.52
1:B:205:THR:HB	1:B:263:ASP:OD2	2.08	0.52
1:C:17:SER:HA	1:C:20:GLU:HG2	1.91	0.52
1:B:212:GLY:HA3	1:B:232:ASN:HD21	1.75	0.52
1:B:198:TYR:CZ	1:B:200:GLY:HA3	2.46	0.51
1:D:55:PRO:O	1:D:56:PRO:C	2.49	0.51
1:B:269:TRP:CZ2	2:B:401:55B:H6	2.46	0.51
1:C:130:PHE:CE2	1:D:26:MET:CE	2.93	0.51
1:C:205:THR:HG22	1:C:206:THR:HG23	1.93	0.51
1:C:212:GLY:HA3	1:C:232:ASN:ND2	2.26	0.51
1:C:17:SER:HA	1:C:20:GLU:CG	2.41	0.50
1:B:225:TYR:O	1:B:228:ILE:HG22	2.11	0.50
1:B:269:TRP:CH2	2:B:401:55B:H6	2.47	0.50
1:D:357:PHE:O	1:D:358:ASN:HB2	2.10	0.49
1:C:191:MET:SD	1:C:194:ILE:HD12	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:MET:HE1	1:A:266:PHE:CE1	2.44	0.49
1:C:269:TRP:CZ2	2:C:401:55B:H1	2.49	0.48
2:D:401:55B:H4	2:D:401:55B:H12	1.44	0.48
1:A:239:ILE:HG23	1:A:250:HIS:HB3	1.96	0.47
1:C:293:HIS:HD2	1:C:367:THR:OG1	1.97	0.47
2:B:401:55B:H8	2:B:401:55B:H9	1.45	0.47
1:A:205:THR:HB	1:A:263:ASP:OD2	2.14	0.47
1:D:269:TRP:CH2	2:D:401:55B:H1	2.50	0.47
1:B:327:ASN:HD21	2:B:401:55B:H1	1.80	0.46
1:D:237:HIS:HD2	5:D:597:HOH:O	1.99	0.46
1:D:198:TYR:CZ	1:D:200:GLY:HA3	2.50	0.46
1:D:157:PHE:CE1	1:D:165:ILE:HA	2.51	0.46
1:D:237:HIS:HE1	5:D:593:HOH:O	1.99	0.46
1:C:149:ALA:HA	1:C:159:LYS:HE3	1.98	0.46
2:D:401:55B:H9	2:D:401:55B:H7	1.69	0.45
1:B:199:ASN:HD22	1:B:199:ASN:N	2.15	0.44
1:B:140:LEU:CD1	1:B:140:LEU:N	2.80	0.44
1:B:224:LYS:HD3	1:B:225:TYR:CE2	2.52	0.44
1:C:274:TRP:HB3	1:C:278:HIS:HB2	1.99	0.44
1:C:322:LEU:HD13	2:C:401:55B:OAC	2.17	0.44
2:A:401:55B:H9	2:A:401:55B:H8	1.50	0.44
1:C:327:ASN:HD21	2:C:401:55B:H6	1.82	0.44
1:B:237:HIS:HD2	5:B:585:HOH:O	2.01	0.43
1:B:234:ASP:O	1:B:252:GLY:HA2	2.18	0.43
1:D:191:MET:CE	1:D:191:MET:HA	2.48	0.43
1:C:157:PHE:CE1	1:C:165:ILE:HA	2.53	0.43
2:D:401:55B:H4	2:D:401:55B:H3	1.38	0.43
1:B:273:ASP:O	1:B:327:ASN:HB3	2.18	0.43
1:C:337:GLU:OE2	1:D:104:LYS:HE2	2.19	0.43
1:A:191:MET:CE	1:A:266:PHE:CE2	3.02	0.43
1:C:158:ASN:HD22	1:C:158:ASN:H	1.67	0.43
1:C:158:ASN:HD22	1:C:158:ASN:N	2.16	0.43
1:D:236:PRO:O	1:D:240:GLN:HG3	2.19	0.43
1:A:149:ALA:HA	1:A:159:LYS:HE3	2.00	0.43
1:D:237:HIS:CD2	5:D:597:HOH:O	2.71	0.43
1:C:193:LYS:HZ2	1:D:15:HIS:CD2	2.31	0.42
1:A:23:LEU:HD21	1:B:358:ASN:HB2	2.01	0.42
1:A:15:HIS:HB3	1:A:17:SER:CB	2.47	0.42
1:B:158:ASN:HD22	1:B:158:ASN:N	2.16	0.42
1:A:228:ILE:HD13	1:A:228:ILE:HG21	1.71	0.42
1:B:207:ILE:HD12	1:B:264:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:TRP:CE2	3:C:402:SAH:H8	2.56	0.41
1:B:135:THR:HA	1:B:140:LEU:HD11	2.02	0.41
1:C:97:LEU:HB3	1:C:105:VAL:CG1	2.50	0.41
1:C:97:LEU:HD11	1:D:306:SER:HB3	2.03	0.41
1:A:212:GLY:HA3	1:A:232:ASN:ND2	2.35	0.41
1:A:126:SER:HA	1:A:189:ILE:HD11	2.03	0.41
1:C:367:THR:HB	1:C:368:ALA:OXT	2.20	0.41
1:C:224:LYS:HD3	1:C:225:TYR:CE2	2.56	0.41
1:B:191:MET:CE	1:B:194:ILE:HD13	2.48	0.41
1:A:269:TRP:CH2	2:A:401:55B:H6	2.56	0.41
1:B:173:HIS:CD2	5:B:543:HOH:O	2.74	0.41
1:A:198:TYR:CZ	1:A:200:GLY:HA3	2.56	0.41
1:C:191:MET:HE3	1:C:268:LYS:HD2	2.03	0.40
1:A:18:ASP:CG	1:B:116:LYS:HE2	2.41	0.40
1:C:266:PHE:CE2	1:C:268:LYS:HB2	2.56	0.40
1:D:283:LEU:HA	1:D:283:LEU:HD23	1.91	0.40
1:D:139:LEU:HD23	1:D:139:LEU:HA	1.93	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	352/368 (96%)	349 (99%)	3 (1%)	0	100 100
1	B	358/368 (97%)	353 (99%)	4 (1%)	1 (0%)	46 29
1	C	352/368 (96%)	347 (99%)	5 (1%)	0	100 100
1	D	359/368 (98%)	352 (98%)	7 (2%)	0	100 100
All	All	1421/1472 (96%)	1401 (99%)	19 (1%)	1 (0%)	56 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/302 (96%)	287 (99%)	4 (1%)	74	65
1	B	297/302 (98%)	291 (98%)	6 (2%)	63	49
1	C	291/302 (96%)	285 (98%)	6 (2%)	61	47
1	D	298/302 (99%)	287 (96%)	11 (4%)	41	23
All	All	1177/1208 (97%)	1150 (98%)	27 (2%)	58	42

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	140	LEU
1	A	272	HIS
1	A	348	ARG
1	B	45	ASP
1	B	147	LYS
1	B	251	LEU
1	B	272	HIS
1	B	336	LYS
1	B	358	ASN
1	C	104	LYS
1	C	105	VAL
1	C	147	LYS
1	C	229	ASN
1	C	269	TRP
1	C	272	HIS
1	D	8	GLU
1	D	15	HIS
1	D	191	MET
1	D	197	MET
1	D	205	THR

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Mol	Chain	Res	Type
1	D	207	ILE
1	D	229	ASN
1	D	251	LEU
1	D	261	LYS
1	D	272	HIS
1	D	277	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	180	ASN
1	A	232	ASN
1	A	237	HIS
1	A	293	HIS
1	B	68	GLN
1	B	158	ASN
1	B	173	HIS
1	B	176	ASN
1	B	180	ASN
1	B	199	ASN
1	B	232	ASN
1	B	237	HIS
1	B	327	ASN
1	B	339	GLN
1	C	158	ASN
1	C	180	ASN
1	C	232	ASN
1	C	237	HIS
1	C	293	HIS
1	C	327	ASN
1	D	15	HIS
1	D	158	ASN
1	D	180	ASN
1	D	229	ASN
1	D	232	ASN
1	D	237	HIS

5.3.3 RNA

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)

17 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	55B	A	401	-	15,15,15	2.76	6 (40%)	18,19,19	4.31	13 (72%)
3	SAH	A	402	-	22,28,28	1.61	3 (13%)	18,40,40	3.30	6 (33%)
4	NO3	A	403	-	1,3,3	0.20	0	0,3,3	0.00	-
4	NO3	A	404	-	1,3,3	0.47	0	0,3,3	0.00	-
4	NO3	A	405	-	1,3,3	0.46	0	0,3,3	0.00	-
2	55B	B	401	-	15,15,15	2.79	7 (46%)	18,19,19	3.63	7 (38%)
3	SAH	B	402	-	22,28,28	0.87	1 (4%)	18,40,40	1.75	3 (16%)
4	NO3	B	403	-	1,3,3	1.32	0	0,3,3	0.00	-
2	55B	C	401	-	15,15,15	2.81	6 (40%)	18,19,19	4.37	11 (61%)
3	SAH	C	402	-	22,28,28	1.44	5 (22%)	18,40,40	3.22	5 (27%)
4	NO3	C	403	-	1,3,3	0.47	0	0,3,3	0.00	-
4	NO3	C	404	-	1,3,3	0.78	0	0,3,3	0.00	-
4	NO3	C	405	-	1,3,3	0.78	0	0,3,3	0.00	-
2	55B	D	401	-	15,15,15	2.54	5 (33%)	18,19,19	4.46	10 (55%)
3	SAH	D	402	-	22,28,28	1.76	5 (22%)	18,40,40	3.88	5 (27%)
4	NO3	D	403	-	1,3,3	0.10	0	0,3,3	0.00	-
4	NO3	D	404	-	1,3,3	0.81	0	0,3,3	0.00	-

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	55B	A	401	-	-	0/8/8/8	0/1/1/1
3	SAH	A	402	-	-	0/7/31/31	0/3/3/3
4	NO3	A	403	-	-	0/0/0/0	0/0/0/0
4	NO3	A	404	-	-	0/0/0/0	0/0/0/0
4	NO3	A	405	-	-	0/0/0/0	0/0/0/0
2	55B	B	401	-	-	0/8/8/8	0/1/1/1
3	SAH	B	402	-	-	0/7/31/31	0/3/3/3
4	NO3	B	403	-	-	0/0/0/0	0/0/0/0
2	55B	C	401	-	-	0/8/8/8	0/1/1/1
3	SAH	C	402	-	-	0/7/31/31	0/3/3/3
4	NO3	C	403	-	-	0/0/0/0	0/0/0/0
4	NO3	C	404	-	-	0/0/0/0	0/0/0/0
4	NO3	C	405	-	-	0/0/0/0	0/0/0/0
2	55B	D	401	-	-	0/8/8/8	0/1/1/1
3	SAH	D	402	-	-	0/7/31/31	0/3/3/3
4	NO3	D	403	-	-	0/0/0/0	0/0/0/0
4	NO3	D	404	-	-	0/0/0/0	0/0/0/0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	SAH	C2'-C1'	-3.43	1.48	1.53
2	A	401	55B	CAL-CAF	-3.25	1.37	1.47
2	B	401	55B	CAL-CAF	-2.95	1.38	1.47
2	D	401	55B	CAL-CAF	-2.93	1.38	1.47
2	C	401	55B	CAL-CAF	-2.35	1.40	1.47
3	C	402	SAH	C2'-C1'	-2.32	1.50	1.53
3	D	402	SAH	O3'-C3'	2.02	1.47	1.43
3	A	402	SAH	O2'-C2'	2.13	1.48	1.43
2	C	401	55B	OAJ-CAA	2.25	1.49	1.42
3	C	402	SAH	C8-N7	2.26	1.39	1.34
2	D	401	55B	CAN-CAM	2.33	1.43	1.40
3	D	402	SAH	C8-N7	2.37	1.39	1.34
3	C	402	SAH	C5-C4	2.39	1.45	1.40
3	C	402	SAH	O4'-C1'	2.42	1.44	1.41
2	B	401	55B	CAH-CAO	2.46	1.43	1.38
2	A	401	55B	CAN-CAM	2.51	1.43	1.40
3	B	402	SAH	C2-N3	2.59	1.36	1.32
2	A	401	55B	CAH-CAO	2.66	1.43	1.38
2	C	401	55B	CAN-CAM	2.91	1.44	1.40
3	D	402	SAH	C5-C4	2.96	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	55B	CAO-CAM	3.21	1.44	1.40
2	B	401	55B	OAJ-CAA	3.25	1.52	1.42
2	B	401	55B	CAO-CAM	3.58	1.45	1.40
2	B	401	55B	CAN-CAM	3.65	1.45	1.40
2	D	401	55B	CAO-CAM	3.82	1.45	1.40
3	C	402	SAH	C2-N3	3.83	1.38	1.32
2	A	401	55B	CAO-CAM	3.98	1.45	1.40
3	A	402	SAH	C2-N3	4.25	1.39	1.32
2	D	401	55B	OAD-CAM	4.27	1.47	1.37
3	D	402	SAH	C2-N3	4.56	1.40	1.32
2	B	401	55B	OAD-CAM	4.70	1.48	1.37
3	A	402	SAH	O4'-C1'	4.84	1.48	1.41
2	A	401	55B	CAF-CAE	5.56	1.50	1.31
2	C	401	55B	OAD-CAM	5.96	1.50	1.37
2	A	401	55B	OAD-CAM	6.01	1.51	1.37
2	B	401	55B	CAF-CAE	6.04	1.52	1.31
2	D	401	55B	CAF-CAE	6.46	1.53	1.31
2	C	401	55B	CAF-CAE	6.55	1.53	1.31

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	402	SAH	N3-C2-N1	-12.55	119.02	128.87
3	C	402	SAH	N3-C2-N1	-11.97	119.47	128.87
2	B	401	55B	CAB-OAK-CAO	-10.50	102.21	117.53
2	D	401	55B	CAA-OAJ-CAN	-9.74	103.32	117.53
3	A	402	SAH	N3-C2-N1	-8.86	121.91	128.87
2	A	401	55B	CAB-OAK-CAO	-8.34	105.35	117.53
2	D	401	55B	CAL-CAF-CAE	-7.25	107.07	127.08
3	A	402	SAH	C1'-N9-C4	-7.11	118.87	126.81
3	D	402	SAH	C4'-O4'-C1'	-6.76	102.48	109.64
2	C	401	55B	CAB-OAK-CAO	-6.61	107.88	117.53
2	C	401	55B	CAL-CAF-CAE	-6.49	109.18	127.08
2	C	401	55B	CAA-OAJ-CAN	-6.19	108.50	117.53
2	A	401	55B	OAJ-CAN-CAG	-6.05	113.79	124.17
2	A	401	55B	CAA-OAJ-CAN	-5.95	108.85	117.53
2	C	401	55B	OAJ-CAN-CAG	-5.43	114.85	124.17
2	C	401	55B	OAK-CAO-CAH	-5.39	114.92	124.17
2	D	401	55B	OAJ-CAN-CAG	-5.33	115.02	124.17
2	C	401	55B	CAO-CAM-CAN	-5.10	111.79	118.75
2	A	401	55B	CAO-CAM-CAN	-4.98	111.95	118.75
2	A	401	55B	OAK-CAO-CAH	-4.78	115.96	124.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	55B	CAL-CAF-CAE	-4.61	114.37	127.08
2	A	401	55B	CAL-CAF-CAE	-4.58	114.44	127.08
2	D	401	55B	OAK-CAO-CAH	-4.45	116.53	124.17
3	C	402	SAH	C1'-N9-C4	-4.40	121.90	126.81
2	D	401	55B	CAB-OAK-CAO	-4.35	111.18	117.53
3	D	402	SAH	O4'-C4'-C5'	-4.31	97.11	108.85
3	B	402	SAH	C1'-N9-C4	-4.27	122.04	126.81
3	A	402	SAH	C4'-O4'-C1'	-4.04	105.36	109.64
2	D	401	55B	CAO-CAM-CAN	-3.78	113.59	118.75
2	B	401	55B	OAK-CAO-CAH	-3.67	117.87	124.17
2	B	401	55B	OAJ-CAN-CAG	-3.65	117.91	124.17
2	B	401	55B	CAO-CAM-CAN	-3.14	114.47	118.75
3	B	402	SAH	N3-C2-N1	-2.43	126.96	128.87
3	A	402	SAH	O4'-C4'-C5'	-2.29	102.62	108.85
3	C	402	SAH	C4'-O4'-C1'	-2.25	107.26	109.64
2	A	401	55B	OAC-CAI-CAE	-2.21	105.54	112.20
2	A	401	55B	OAD-CAM-CAN	2.10	123.91	119.28
3	C	402	SAH	N6-C6-N1	2.16	122.13	118.52
2	C	401	55B	CAG-CAN-CAM	2.16	122.81	120.57
2	A	401	55B	OAD-CAM-CAO	2.18	124.10	119.28
3	A	402	SAH	C2-N1-C6	2.23	122.75	118.77
3	C	402	SAH	C2-N1-C6	2.33	122.93	118.77
2	C	401	55B	OAD-CAM-CAO	2.37	124.52	119.28
2	D	401	55B	OAD-CAM-CAO	2.40	124.57	119.28
2	A	401	55B	CAH-CAO-CAM	2.93	123.60	120.57
2	D	401	55B	CAH-CAO-CAM	3.17	123.86	120.57
2	A	401	55B	CAG-CAN-CAM	3.57	124.27	120.57
2	C	401	55B	CAH-CAO-CAM	3.58	124.28	120.57
3	B	402	SAH	N6-C6-N1	4.00	125.22	118.52
3	D	402	SAH	N6-C6-N1	4.16	125.50	118.52
3	D	402	SAH	C2-N1-C6	4.55	126.88	118.77
2	B	401	55B	OAJ-CAN-CAM	5.02	119.57	114.47
2	D	401	55B	OAK-CAO-CAM	5.05	119.60	114.47
3	A	402	SAH	N6-C6-N1	5.27	127.36	118.52
2	B	401	55B	OAK-CAO-CAM	5.32	119.87	114.47
2	A	401	55B	OAK-CAO-CAM	5.78	120.34	114.47
2	C	401	55B	OAK-CAO-CAM	6.23	120.80	114.47
2	A	401	55B	OAJ-CAN-CAM	7.34	121.93	114.47
2	C	401	55B	OAJ-CAN-CAM	7.74	122.33	114.47
2	D	401	55B	OAJ-CAN-CAM	8.42	123.03	114.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	55B	3	0
2	B	401	55B	4	0
2	C	401	55B	4	0
3	C	402	SAH	1	0
2	D	401	55B	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	354/368 (96%)	-0.55	3 (0%)	87 85	5, 12, 26, 70	0
1	B	360/368 (97%)	-0.44	6 (1%)	73 69	6, 16, 36, 69	0
1	C	354/368 (96%)	-0.49	6 (1%)	73 69	6, 14, 32, 67	0
1	D	361/368 (98%)	-0.40	5 (1%)	78 74	7, 18, 37, 69	0
All	All	1429/1472 (97%)	-0.47	20 (1%)	78 74	5, 15, 34, 70	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	368	ALA	6.7
1	A	15	HIS	5.9
1	C	56	PRO	5.3
1	C	368	ALA	5.3
1	D	55	PRO	5.2
1	D	57	SER	4.8
1	B	56	PRO	4.1
1	D	56	PRO	3.7
1	A	368	ALA	3.5
1	C	15	HIS	3.5
1	D	368	ALA	3.4
1	B	100	LEU	3.3
1	B	103	GLY	3.3
1	C	103	GLY	3.2
1	B	54	VAL	2.8
1	A	16	SER	2.7
1	C	57	SER	2.7
1	D	103	GLY	2.4
1	C	293	HIS	2.1
1	B	72	THR	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	55B	C	401	15/15	0.78	0.25	12.06	19,34,48,60	0
2	55B	D	401	15/15	0.71	0.24	11.54	25,43,50,51	0
4	NO3	D	404	4/4	0.89	0.20	9.74	27,36,37,38	0
2	55B	B	401	15/15	0.87	0.24	9.66	18,33,72,80	0
2	55B	A	401	15/15	0.77	0.19	7.95	19,39,45,47	0
4	NO3	A	404	4/4	0.97	0.16	7.03	24,24,28,31	0
4	NO3	C	403	4/4	0.94	0.18	6.59	31,33,36,44	0
4	NO3	D	403	4/4	0.98	0.11	4.30	22,24,26,28	0
4	NO3	B	403	4/4	0.90	0.13	4.06	41,42,45,48	0
4	NO3	A	405	4/4	0.94	0.12	2.23	21,32,36,39	0
4	NO3	C	404	4/4	0.90	0.14	1.91	29,31,32,36	0
4	NO3	A	403	4/4	0.94	0.09	1.28	29,29,30,30	0
4	NO3	C	405	4/4	0.97	0.10	0.49	33,33,34,35	0
3	SAH	A	402	26/26	0.97	0.08	-0.01	7,8,12,14	0
3	SAH	D	402	26/26	0.95	0.07	-0.46	13,16,19,19	0
3	SAH	C	402	26/26	0.97	0.07	-0.47	9,12,14,15	0
3	SAH	B	402	26/26	0.97	0.06	-0.59	11,13,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.