Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:16 PM GMT

PDB ID	:	1ESM
Title	:	STRUCTURAL BASIS FOR THE FEEDBACK REGULATION OF ES-CHERICHIA COLI PANTOTHENATE KINASE BY COENZYME A
Authors	:	Yun, M.; Park, C.G.; Kim, J.Y.; Rock, C.O.; Jackowski, S.; Park, H.W.
Deposited on	:	2000-04-10
Resolution	:	2.50 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.

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
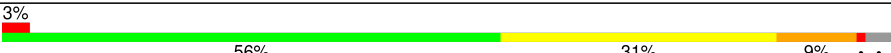*X-RAY DIFFRACTION*
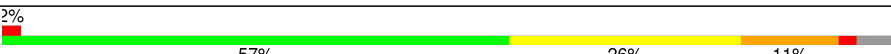
The reported resolution of this entry is 2.50 Å.

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.
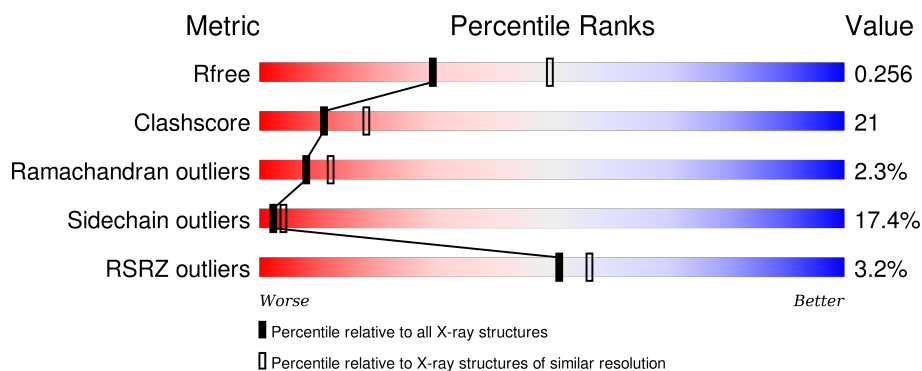
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	316	5% 57% 32% 8% ··
1	B	316	3% 56% 29% 11% ··
1	C	316	3% 56% 31% 9% ··
1	D	316	2% 57% 26% 11% ··

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10473 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 PANTOTHENATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	Se	0	0	0
			2528	1623	434	465	6			
1	B	307	Total	C	N	O	Se	0	0	0
			2495	1603	427	459	6			
1	C	307	Total	C	N	O	Se	0	0	0
			2491	1599	428	458	6			
1	D	303	Total	C	N	O	Se	0	0	0
			2466	1588	421	451	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
A	29	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
A	142	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
A	153	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
A	208	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
A	275	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
B	9	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
B	29	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
B	142	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
B	153	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
B	208	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
B	275	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
C	9	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
C	29	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
C	142	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
C	153	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
C	208	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
C	275	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
D	9	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
D	29	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
D	142	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	153	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
D	208	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3
D	275	MSE	MET	MODIFIED RESIDUE	UNP P0A6I3

• Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).
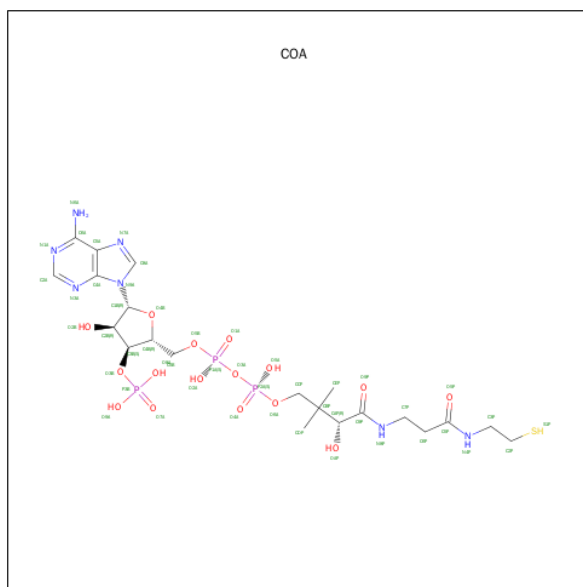
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total	O	0	0
			67	67		
3	B	78	Total	O	0	0
			78	78		
3	C	72	Total	O	0	0
			72	72		
3	D	84	Total	O	0	0
			84	84		

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: PANTOTHENATE KINASE
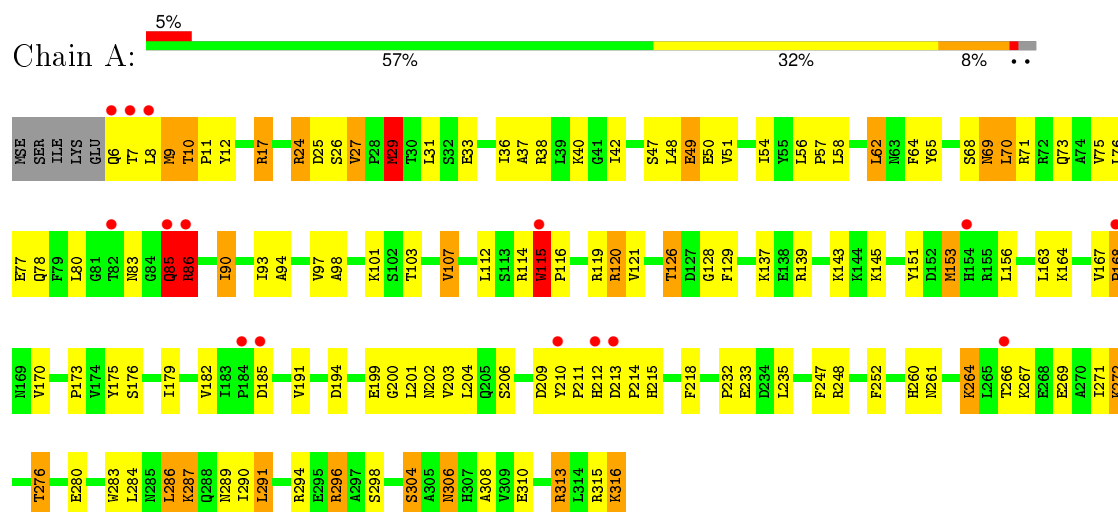
- Molecule 1: PANTOTHENATE KINASE

- Molecule 1: PANTOTHENATE KINASE

• Molecule 1: PANTOTHENATE KINASE

Chain D:
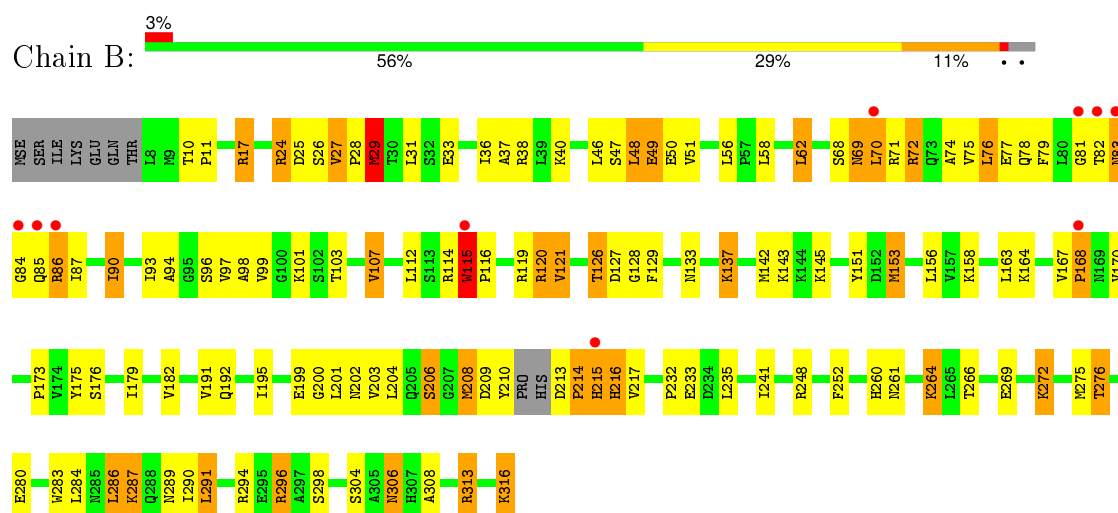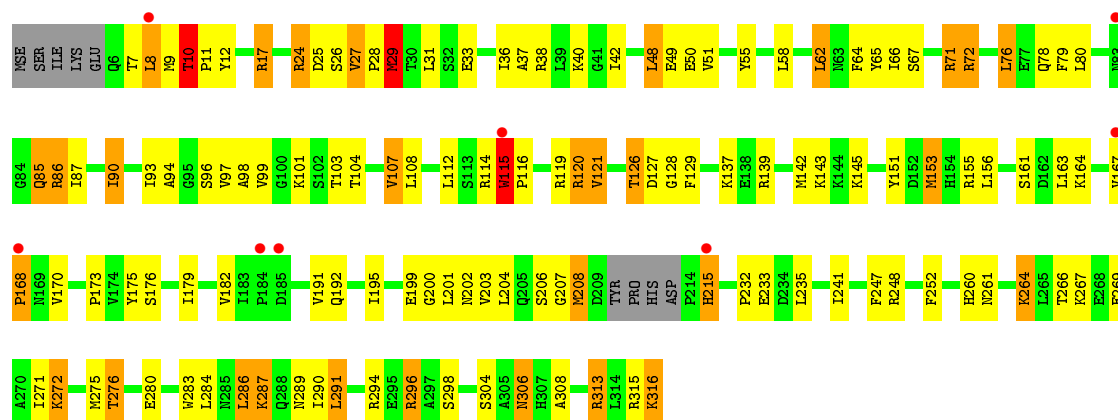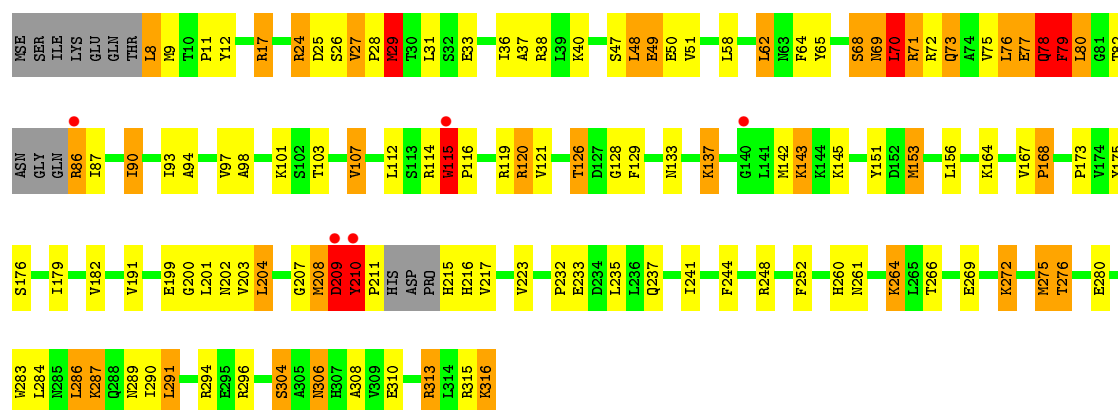
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.00Å 71.24Å 87.68Å 102.44° 89.48° 93.23°	Depositor
Resolution (Å)	50.00 – 2.50 37.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	81.4 (50.00-2.50) 78.0 (37.69-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.93 (at 2.51Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.201 , 0.259 0.204 , 0.256	Depositor DCC
R_{free} test set	2071 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 61.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Outliers	0 of 43148 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10473	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.49	3/2581 (0.1%)	0.71	4/3494 (0.1%)
1	B	0.51	3/2545 (0.1%)	0.73	4/3442 (0.1%)
1	C	0.49	3/2540 (0.1%)	0.72	5/3434 (0.1%)
1	D	0.51	4/2515 (0.2%)	0.75	8/3400 (0.2%)
All	All	0.50	13/10181 (0.1%)	0.73	21/13770 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	MSE	CG-SE	-6.41	1.73	1.95
1	C	153	MSE	CG-SE	-6.22	1.74	1.95
1	D	153	MSE	CG-SE	-6.16	1.74	1.95
1	B	29	MSE	CG-SE	-6.07	1.74	1.95
1	C	29	MSE	CG-SE	-5.97	1.75	1.95
1	A	153	MSE	CG-SE	-5.96	1.75	1.95
1	D	29	MSE	CG-SE	-5.83	1.75	1.95
1	B	208	MSE	CG-SE	-5.65	1.76	1.95
1	A	29	MSE	CG-SE	-5.55	1.76	1.95
1	D	208	MSE	CG-SE	-5.45	1.76	1.95
1	A	9	MSE	CG-SE	-5.14	1.77	1.95
1	D	275	MSE	CG-SE	-5.08	1.78	1.95
1	C	208	MSE	CG-SE	-5.05	1.78	1.95

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	THR	N-CA-C	-8.29	88.62	111.00
1	C	10	THR	N-CA-C	-7.42	90.96	111.00
1	D	208	MSE	CA-CB-CG	-7.09	101.25	113.30
1	A	143	LYS	N-CA-C	-6.75	92.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	LYS	N-CA-C	-6.73	92.83	111.00
1	D	208	MSE	CA-C-N	-6.63	102.60	117.20
1	D	143	LYS	N-CA-C	-6.60	93.18	111.00
1	B	143	LYS	N-CA-C	-6.52	93.41	111.00
1	B	153	MSE	CA-CB-CG	-6.26	102.66	113.30
1	B	29	MSE	CB-CG-SE	-6.20	94.12	112.70
1	C	153	MSE	CA-CB-CG	-6.02	103.07	113.30
1	D	142	MSE	CB-CG-SE	-5.94	94.88	112.70
1	D	78	GLN	N-CA-C	-5.88	95.12	111.00
1	D	153	MSE	CA-CB-CG	-5.80	103.43	113.30
1	C	29	MSE	CB-CG-SE	-5.76	95.42	112.70
1	D	29	MSE	CB-CG-SE	-5.74	95.48	112.70
1	B	142	MSE	CB-CG-SE	-5.53	96.11	112.70
1	C	142	MSE	CB-CG-SE	-5.33	96.72	112.70
1	A	29	MSE	CB-CG-SE	-5.29	96.81	112.70
1	A	153	MSE	CA-CB-CG	-5.18	104.49	113.30
1	D	79	PHE	N-CA-CB	5.02	119.63	110.60

There are no chirality outliers.

There are no planarity outliers.

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	2528	0	2540	107	0
1	B	2495	0	2510	135	0
1	C	2491	0	2513	107	0
1	D	2466	0	2488	116	0
2	A	48	0	32	0	0
2	B	48	0	32	0	0
2	C	48	0	32	0	0
2	D	48	0	32	0	0
3	A	67	0	0	1	0
3	B	78	0	0	3	0
3	C	72	0	0	0	0
3	D	84	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10473	0	10179	425	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 21.

All (425) 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:29:MSE:HE2	1:B:31:LEU:HB2	1.19	1.14
1:D:210:TYR:HB3	1:D:211:PRO:CD	1.81	1.10
1:C:29:MSE:HE2	1:C:31:LEU:HB2	1.20	1.09
1:D:29:MSE:HE2	1:D:31:LEU:HB2	1.17	1.09
1:A:29:MSE:HE2	1:A:31:LEU:HB2	1.13	1.09
1:B:215:HIS:CD2	1:B:216:HIS:H	1.71	1.08
1:D:210:TYR:HB3	1:D:211:PRO:HD2	1.05	1.02
1:A:65:TYR:CE2	1:B:75:VAL:HG21	1.96	1.00
1:D:75:VAL:O	1:D:78:GLN:O	1.80	1.00
1:D:29:MSE:HE1	1:D:51:VAL:HG11	1.43	0.98
1:B:85:GLN:HA	1:B:87:ILE:HD13	1.47	0.96
1:B:29:MSE:HE1	1:B:51:VAL:HG11	1.43	0.95
1:C:29:MSE:HE1	1:C:51:VAL:HG11	1.51	0.92
1:A:29:MSE:HE1	1:A:51:VAL:HG11	1.50	0.91
1:C:85:GLN:HE22	1:C:192:GLN:HE22	1.21	0.89
1:D:210:TYR:CB	1:D:211:PRO:HD2	1.99	0.88
1:A:86:ARG:HG3	1:A:86:ARG:O	1.73	0.87
1:A:86:ARG:HH22	1:A:194:ASP:HA	1.41	0.86
1:A:29:MSE:CE	1:A:31:LEU:HB2	2.05	0.85
1:D:76:LEU:O	1:D:80:LEU:HB2	1.82	0.80
1:D:261:ASN:HA	1:D:264:LYS:HE2	1.65	0.79
1:A:11:PRO:HG3	1:B:215:HIS:HB2	1.65	0.79
1:B:215:HIS:CG	1:B:216:HIS:H	1.98	0.79
1:C:72:ARG:CG	1:C:72:ARG:HH11	1.95	0.78
1:C:161:SER:HG	1:D:8:LEU:N	1.82	0.78
1:C:261:ASN:HA	1:C:264:LYS:HE2	1.66	0.78
1:D:211:PRO:HB2	1:D:216:HIS:HD2	1.47	0.78
1:B:75:VAL:HG22	3:B:529:HOH:O	1.83	0.77
1:A:261:ASN:HA	1:A:264:LYS:HE2	1.67	0.77
1:B:261:ASN:HA	1:B:264:LYS:HE2	1.67	0.77
1:C:29:MSE:CE	1:C:31:LEU:HB2	2.11	0.76
1:A:213:ASP:C	1:A:215:HIS:H	1.89	0.76
1:A:126:THR:HB	1:A:200:GLY:HA3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:MSE:CE	1:B:31:LEU:HB2	2.10	0.75
1:C:126:THR:HB	1:C:200:GLY:HA3	1.68	0.75
1:D:11:PRO:O	1:D:316:LYS:HG2	1.87	0.75
1:C:8:LEU:HD22	1:C:8:LEU:O	1.87	0.74
1:B:213:ASP:O	1:B:214:PRO:O	2.06	0.73
1:A:266:THR:HG23	1:A:269:GLU:H	1.53	0.73
1:C:266:THR:HG23	1:C:269:GLU:H	1.52	0.73
1:B:266:THR:HG23	1:B:269:GLU:H	1.54	0.73
1:D:266:THR:HG23	1:D:269:GLU:H	1.54	0.73
1:C:85:GLN:HE22	1:C:192:GLN:NE2	1.86	0.72
1:C:64:PHE:CD2	1:D:79:PHE:HB2	2.24	0.72
1:A:11:PRO:CD	1:B:215:HIS:HB2	2.20	0.72
1:B:85:GLN:HA	1:B:87:ILE:CD1	2.19	0.72
1:C:85:GLN:HG3	1:C:86:ARG:N	2.05	0.71
1:D:29:MSE:CE	1:D:31:LEU:HB2	2.08	0.71
1:C:11:PRO:HG3	1:D:215:HIS:HA	1.72	0.71
1:B:126:THR:HB	1:B:200:GLY:HA3	1.73	0.71
1:D:286:LEU:HD22	1:D:291:LEU:HD22	1.73	0.71
1:B:286:LEU:HD22	1:B:291:LEU:HD22	1.73	0.70
1:C:286:LEU:HD22	1:C:291:LEU:HD22	1.72	0.70
1:A:11:PRO:O	1:A:316:LYS:HG2	1.91	0.70
1:B:167:VAL:HG13	1:B:168:PRO:HD2	1.74	0.69
1:D:79:PHE:O	1:D:79:PHE:CD2	2.45	0.69
1:C:11:PRO:O	1:C:316:LYS:HG2	1.92	0.69
1:A:139:ARG:HB3	1:D:264:LYS:NZ	2.07	0.68
1:A:11:PRO:CG	1:B:215:HIS:HB2	2.22	0.68
1:C:266:THR:HG22	1:C:269:GLU:CD	2.14	0.68
1:B:126:THR:HG21	1:B:202:ASN:OD1	1.94	0.68
1:A:86:ARG:CG	1:A:86:ARG:O	2.41	0.68
1:A:11:PRO:HD3	1:B:215:HIS:HB2	1.75	0.68
1:D:126:THR:HG21	1:D:202:ASN:OD1	1.93	0.67
1:A:266:THR:HG22	1:A:269:GLU:CD	2.14	0.67
1:C:126:THR:HG21	1:C:202:ASN:OD1	1.94	0.67
1:B:11:PRO:O	1:B:316:LYS:HG2	1.93	0.67
1:C:306:ASN:ND2	1:C:308:ALA:HB3	2.09	0.67
1:D:126:THR:HB	1:D:200:GLY:HA3	1.74	0.67
1:A:126:THR:HG21	1:A:202:ASN:OD1	1.95	0.67
1:C:208:MSE:HA	1:D:209:ASP:OD1	1.93	0.66
1:B:164:LYS:HE2	3:B:658:HOH:O	1.96	0.66
1:B:266:THR:HG22	1:B:269:GLU:CD	2.15	0.66
1:C:9:MSE:HA	1:D:217:VAL:HG21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:SER:O	1:C:208:MSE:HG2	1.94	0.66
1:D:25:ASP:CG	1:D:26:SER:H	1.98	0.66
1:B:213:ASP:N	1:B:214:PRO:HD2	2.10	0.66
1:C:64:PHE:HD2	1:D:79:PHE:HB2	1.60	0.66
1:A:286:LEU:HD22	1:A:291:LEU:HD22	1.76	0.66
1:A:24:ARG:NH1	1:A:27:VAL:O	2.28	0.65
1:C:24:ARG:O	1:C:27:VAL:HG13	1.97	0.65
1:A:9:MSE:HB2	1:B:217:VAL:HB	1.78	0.65
1:B:214:PRO:HG2	1:B:216:HIS:CE1	2.32	0.65
1:B:86:ARG:HG2	1:B:86:ARG:O	1.96	0.65
1:C:72:ARG:HG2	1:C:72:ARG:HH11	1.60	0.65
1:B:115:TRP:CE3	1:B:115:TRP:C	2.70	0.65
1:B:115:TRP:HB3	1:B:116:PRO:HD3	1.79	0.65
1:B:85:GLN:O	1:B:87:ILE:HD12	1.97	0.64
1:B:306:ASN:ND2	1:B:308:ALA:HB3	2.12	0.64
1:C:85:GLN:NE2	1:C:192:GLN:HE22	1.94	0.64
1:A:25:ASP:CG	1:A:26:SER:H	1.97	0.64
1:D:266:THR:HG22	1:D:269:GLU:CD	2.17	0.64
1:C:62:LEU:O	1:C:66:ILE:HG13	1.97	0.64
1:A:115:TRP:C	1:A:115:TRP:CE3	2.71	0.64
1:C:115:TRP:HB3	1:C:116:PRO:HD3	1.78	0.64
1:C:72:ARG:NH1	1:C:72:ARG:HG2	2.12	0.64
1:D:153:MSE:CG	1:D:156:LEU:HB3	2.28	0.63
1:A:86:ARG:NH2	1:A:194:ASP:HA	2.13	0.63
1:D:24:ARG:NH1	1:D:27:VAL:O	2.27	0.63
1:C:115:TRP:C	1:C:115:TRP:CE3	2.72	0.63
1:B:215:HIS:CG	1:B:216:HIS:N	2.66	0.63
1:A:115:TRP:HB3	1:A:116:PRO:HD3	1.80	0.62
1:C:25:ASP:CG	1:C:26:SER:H	2.01	0.62
1:C:201:LEU:HD22	1:C:290:ILE:HD11	1.80	0.62
1:B:75:VAL:HG23	1:B:76:LEU:N	2.14	0.62
1:D:115:TRP:HB3	1:D:116:PRO:HD3	1.80	0.62
1:C:207:GLY:O	1:D:209:ASP:OD1	2.18	0.62
1:D:115:TRP:C	1:D:115:TRP:CE3	2.73	0.61
1:A:306:ASN:ND2	1:A:308:ALA:HB3	2.15	0.61
1:A:167:VAL:HG13	1:A:168:PRO:HD2	1.81	0.61
1:D:306:ASN:ND2	1:D:308:ALA:HB3	2.15	0.61
1:A:201:LEU:HD22	1:A:290:ILE:HD11	1.83	0.61
1:D:167:VAL:HG13	1:D:168:PRO:HD2	1.81	0.61
1:D:313:ARG:HH11	1:D:313:ARG:HG2	1.66	0.61
1:C:9:MSE:HB2	1:D:217:VAL:HB	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:THR:O	1:B:107:VAL:HG12	2.01	0.60
1:A:65:TYR:HE2	1:B:75:VAL:HG21	1.62	0.60
1:A:139:ARG:HB3	1:D:264:LYS:HZ2	1.65	0.59
1:C:29:MSE:HE2	1:C:31:LEU:CB	2.14	0.59
1:A:94:ALA:HB2	1:A:203:VAL:CG2	2.32	0.59
1:B:37:ALA:HA	1:B:40:LYS:HD2	1.84	0.59
1:C:64:PHE:HE2	1:D:79:PHE:HA	1.68	0.59
1:B:115:TRP:CE3	1:B:115:TRP:O	2.56	0.59
1:C:94:ALA:HB2	1:C:203:VAL:CG2	2.32	0.58
1:A:213:ASP:C	1:A:215:HIS:N	2.55	0.58
1:D:79:PHE:O	1:D:79:PHE:CG	2.56	0.58
1:D:24:ARG:O	1:D:27:VAL:HG13	2.03	0.58
1:C:313:ARG:HG2	1:C:313:ARG:HH11	1.68	0.58
1:C:167:VAL:HG13	1:C:168:PRO:HD2	1.85	0.58
1:D:8:LEU:N	1:D:8:LEU:HD12	2.18	0.58
1:C:276:THR:O	1:C:280:GLU:HG3	2.03	0.58
1:B:33:GLU:HG3	1:B:48:LEU:HD13	1.86	0.58
1:A:232:PRO:HD2	1:A:235:LEU:HD12	1.84	0.58
1:A:24:ARG:O	1:A:27:VAL:HG13	2.03	0.58
1:A:9:MSE:HA	1:B:217:VAL:HG21	1.86	0.58
1:B:94:ALA:HB2	1:B:203:VAL:CG2	2.34	0.57
1:C:37:ALA:HA	1:C:40:LYS:HD2	1.86	0.57
1:B:201:LEU:HD22	1:B:290:ILE:HD11	1.85	0.57
1:B:25:ASP:CG	1:B:26:SER:H	2.07	0.57
1:D:94:ALA:HB2	1:D:203:VAL:CG2	2.34	0.57
1:A:115:TRP:CB	1:A:116:PRO:HD3	2.35	0.57
1:B:115:TRP:CB	1:B:116:PRO:HD3	2.35	0.57
1:A:272:LYS:O	1:A:276:THR:HG23	2.04	0.57
1:D:241:ILE:HD11	1:D:275:MSE:HG3	1.86	0.57
1:A:153:MSE:CG	1:A:156:LEU:HB3	2.34	0.57
1:A:64:PHE:HE2	1:B:79:PHE:HA	1.68	0.56
1:C:115:TRP:CB	1:C:116:PRO:HD3	2.34	0.56
1:B:24:ARG:O	1:B:27:VAL:HG13	2.04	0.56
1:B:29:MSE:HE1	1:B:51:VAL:CG1	2.28	0.56
1:B:209:ASP:O	1:B:210:TYR:CB	2.53	0.56
1:A:211:PRO:HB2	1:D:143:LYS:HD2	1.87	0.56
1:A:70:LEU:HA	1:A:73:GLN:HE21	1.71	0.56
1:A:213:ASP:N	1:A:214:PRO:CD	2.67	0.56
1:D:232:PRO:HD2	1:D:235:LEU:HD12	1.88	0.56
1:C:103:THR:O	1:C:107:VAL:HG12	2.06	0.56
1:D:153:MSE:HG2	1:D:156:LEU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ARG:HH21	1:B:87:ILE:HG21	1.71	0.56
1:D:25:ASP:CG	1:D:26:SER:N	2.59	0.56
1:B:313:ARG:HH11	1:B:313:ARG:HG2	1.69	0.56
1:D:37:ALA:HA	1:D:40:LYS:HD2	1.87	0.56
1:D:272:LYS:O	1:D:276:THR:HG23	2.06	0.56
1:B:29:MSE:CE	1:B:51:VAL:HG11	2.28	0.56
1:A:313:ARG:HH11	1:A:313:ARG:HG2	1.70	0.56
1:D:201:LEU:HD22	1:D:290:ILE:HD11	1.88	0.56
1:D:115:TRP:CB	1:D:116:PRO:HD3	2.36	0.55
1:A:69:ASN:C	1:A:69:ASN:HD22	2.09	0.55
1:B:215:HIS:C	1:B:216:HIS:O	2.44	0.55
1:A:73:GLN:O	1:A:77:GLU:HG3	2.07	0.55
1:C:25:ASP:CG	1:C:26:SER:N	2.60	0.55
1:A:103:THR:O	1:A:107:VAL:HG12	2.07	0.55
1:A:185:ASP:HB2	3:A:665:HOH:O	2.06	0.55
1:D:77:GLU:OE1	1:D:87:ILE:HD12	2.06	0.55
1:C:115:TRP:O	1:C:115:TRP:CE3	2.60	0.54
1:B:276:THR:O	1:B:280:GLU:HG3	2.06	0.54
1:A:90:ILE:HD11	1:A:164:LYS:HG3	1.89	0.54
1:B:153:MSE:CG	1:B:156:LEU:HB3	2.37	0.54
1:A:25:ASP:CG	1:A:26:SER:N	2.61	0.54
1:A:115:TRP:O	1:A:115:TRP:CE3	2.61	0.54
1:B:272:LYS:O	1:B:276:THR:HG23	2.08	0.54
1:C:232:PRO:HD2	1:C:235:LEU:HD12	1.89	0.54
1:B:209:ASP:HB3	1:B:296:ARG:HH21	1.72	0.54
1:A:11:PRO:HG3	1:B:215:HIS:CB	2.34	0.54
1:D:115:TRP:CE3	1:D:115:TRP:O	2.62	0.53
1:C:90:ILE:HD11	1:C:164:LYS:HG3	1.90	0.53
1:D:103:THR:O	1:D:107:VAL:HG12	2.08	0.53
1:B:85:GLN:O	1:B:86:ARG:HB3	2.09	0.53
1:A:153:MSE:HG3	1:A:156:LEU:HB3	1.90	0.53
1:C:272:LYS:O	1:C:276:THR:HG23	2.08	0.53
1:A:37:ALA:HA	1:A:40:LYS:HD2	1.91	0.53
1:C:153:MSE:HG3	1:C:156:LEU:HB3	1.90	0.53
1:A:33:GLU:HG3	1:A:48:LEU:HD13	1.91	0.53
1:D:69:ASN:O	1:D:71:ARG:N	2.42	0.53
1:B:153:MSE:HG3	1:B:156:LEU:HB3	1.90	0.53
1:B:68:SER:O	1:B:70:LEU:HD22	2.09	0.53
1:B:90:ILE:HD11	1:B:164:LYS:HG3	1.90	0.52
1:B:241:ILE:HD11	1:B:275:MSE:HG3	1.91	0.52
1:B:232:PRO:HD2	1:B:235:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:THR:HG22	1:D:215:HIS:NE2	2.23	0.52
1:C:24:ARG:NH1	1:C:27:VAL:O	2.34	0.52
1:C:97:VAL:O	1:C:98:ALA:HB3	2.09	0.52
1:A:115:TRP:CG	1:A:116:PRO:HD3	2.44	0.52
1:A:276:THR:O	1:A:280:GLU:HG3	2.10	0.52
1:A:97:VAL:O	1:A:98:ALA:HB3	2.10	0.52
1:C:208:MSE:CA	1:D:209:ASP:OD1	2.58	0.52
1:D:153:MSE:HG3	1:D:156:LEU:HB3	1.91	0.52
1:B:24:ARG:NH1	1:B:27:VAL:O	2.33	0.52
1:A:8:LEU:HD22	1:B:158:LYS:HD2	1.91	0.52
1:A:29:MSE:CE	1:A:51:VAL:HG11	2.31	0.51
1:B:115:TRP:C	1:B:115:TRP:CD2	2.84	0.51
1:C:115:TRP:CG	1:C:116:PRO:HD3	2.45	0.51
1:B:97:VAL:O	1:B:98:ALA:HB3	2.10	0.51
1:D:211:PRO:HB2	1:D:216:HIS:CD2	2.38	0.51
1:C:153:MSE:CG	1:C:156:LEU:HB3	2.40	0.51
1:D:252:PHE:O	1:D:260:HIS:HD2	1.93	0.51
1:D:97:VAL:O	1:D:98:ALA:HB3	2.11	0.51
1:B:25:ASP:CG	1:B:26:SER:N	2.64	0.51
1:B:77:GLU:O	1:B:81:GLY:N	2.44	0.51
1:D:65:TYR:CD2	1:D:70:LEU:HD23	2.46	0.51
1:B:252:PHE:O	1:B:260:HIS:HD2	1.94	0.51
1:D:207:GLY:HA2	1:D:210:TYR:HB2	1.92	0.51
1:C:29:MSE:HG3	1:C:31:LEU:H	1.75	0.50
1:D:29:MSE:CE	1:D:51:VAL:HG11	2.29	0.50
1:B:115:TRP:CG	1:B:116:PRO:HD3	2.45	0.50
1:B:68:SER:O	1:B:69:ASN:C	2.50	0.50
1:A:76:LEU:O	1:A:80:LEU:HG	2.12	0.50
1:A:139:ARG:O	1:D:260:HIS:HE1	1.95	0.50
1:D:207:GLY:O	1:D:210:TYR:HD1	1.94	0.50
1:C:33:GLU:HG3	1:C:48:LEU:HD13	1.92	0.50
1:D:112:LEU:O	1:D:119:ARG:HD2	2.11	0.50
1:B:85:GLN:C	1:B:87:ILE:HD12	2.32	0.50
1:B:85:GLN:C	1:B:87:ILE:H	2.14	0.50
1:C:64:PHE:HE2	1:D:79:PHE:CA	2.25	0.49
1:B:74:ALA:C	1:B:78:GLN:HE21	2.15	0.49
1:B:85:GLN:C	1:B:87:ILE:N	2.65	0.49
1:D:276:THR:O	1:D:280:GLU:HG3	2.12	0.49
1:A:283:TRP:CZ2	1:A:287:LYS:HD2	2.47	0.49
1:A:85:GLN:O	1:A:86:ARG:HB3	2.12	0.49
1:A:252:PHE:O	1:A:260:HIS:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:GLY:C	1:D:210:TYR:HB2	2.33	0.49
1:A:29:MSE:HG3	1:A:31:LEU:H	1.78	0.49
1:A:58:LEU:O	1:A:62:LEU:HB2	2.13	0.49
1:C:252:PHE:O	1:C:260:HIS:HD2	1.96	0.49
1:B:58:LEU:O	1:B:62:LEU:HB2	2.12	0.49
1:C:11:PRO:CG	1:D:215:HIS:HA	2.41	0.48
1:A:8:LEU:CD2	1:B:158:LYS:HD2	2.42	0.48
1:A:213:ASP:O	1:A:215:HIS:N	2.47	0.48
1:D:313:ARG:HG2	1:D:313:ARG:NH1	2.28	0.48
1:C:29:MSE:HE1	1:C:51:VAL:CG1	2.34	0.48
1:A:29:MSE:HE2	1:A:31:LEU:CB	2.09	0.48
1:C:115:TRP:C	1:C:115:TRP:CD2	2.87	0.48
1:D:90:ILE:HD11	1:D:164:LYS:HG3	1.96	0.48
1:B:233:GLU:OE1	1:B:287:LYS:HE3	2.14	0.47
1:D:115:TRP:C	1:D:115:TRP:CD2	2.87	0.47
1:B:112:LEU:O	1:B:119:ARG:HD2	2.13	0.47
1:B:74:ALA:O	1:B:78:GLN:HG2	2.13	0.47
1:B:176:SER:HB3	1:B:179:ILE:HG12	1.96	0.47
1:D:33:GLU:HG3	1:D:48:LEU:HD13	1.95	0.47
1:C:129:PHE:CZ	1:C:173:PRO:HD2	2.49	0.47
1:B:313:ARG:NH1	1:B:313:ARG:HG2	2.30	0.47
1:A:112:LEU:O	1:A:119:ARG:HD2	2.14	0.47
1:D:64:PHE:O	1:D:68:SER:HB2	2.14	0.47
1:D:115:TRP:CG	1:D:116:PRO:HD3	2.49	0.47
1:A:75:VAL:HG22	1:A:76:LEU:N	2.29	0.47
1:A:129:PHE:CZ	1:A:173:PRO:HD2	2.49	0.47
1:D:266:THR:HG22	1:D:269:GLU:HB2	1.96	0.47
1:B:316:LYS:H	1:B:316:LYS:HG2	1.54	0.47
1:B:137:LYS:NZ	3:B:760:HOH:O	2.47	0.47
1:C:233:GLU:OE1	1:C:287:LYS:HE3	2.15	0.47
1:D:68:SER:O	1:D:70:LEU:N	2.48	0.47
1:A:209:ASP:OD1	1:A:296:ARG:NH2	2.47	0.47
1:B:126:THR:CG2	1:B:151:TYR:CE2	2.98	0.47
1:D:233:GLU:OE1	1:D:287:LYS:HE3	2.15	0.47
1:A:85:GLN:O	1:A:86:ARG:CB	2.63	0.46
1:A:115:TRP:CD2	1:A:115:TRP:C	2.87	0.46
1:B:153:MSE:O	1:B:153:MSE:HG2	2.15	0.46
1:C:64:PHE:CE2	1:D:79:PHE:HB2	2.49	0.46
1:D:291:LEU:HD11	1:D:294:ARG:NH1	2.30	0.46
1:D:207:GLY:CA	1:D:210:TYR:HB2	2.45	0.46
1:B:215:HIS:CD2	1:B:216:HIS:N	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LEU:O	1:C:119:ARG:HD2	2.15	0.46
1:B:68:SER:O	1:B:70:LEU:N	2.48	0.46
1:B:206:SER:C	1:B:208:MSE:H	2.17	0.46
1:A:153:MSE:HG2	1:A:156:LEU:HB3	1.98	0.46
1:A:316:LYS:H	1:A:316:LYS:HG2	1.54	0.46
1:C:313:ARG:NH1	1:C:313:ARG:HG2	2.29	0.46
1:C:71:ARG:HE	1:C:71:ARG:HB2	1.41	0.46
1:B:75:VAL:HG23	1:B:76:LEU:H	1.81	0.46
1:C:215:HIS:N	1:C:215:HIS:CD2	2.84	0.46
1:A:212:HIS:N	1:A:214:PRO:HD3	2.31	0.45
1:A:128:GLY:HA2	1:A:175:TYR:HB2	1.98	0.45
1:B:96:SER:O	1:B:99:VAL:HG12	2.15	0.45
1:B:266:THR:HG22	1:B:269:GLU:HB2	1.99	0.45
1:C:208:MSE:HB3	1:D:209:ASP:OD1	2.16	0.45
1:D:65:TYR:HD2	1:D:70:LEU:HD23	1.80	0.45
1:C:58:LEU:O	1:C:62:LEU:HB2	2.16	0.45
1:D:129:PHE:CZ	1:D:173:PRO:HD2	2.51	0.45
1:D:208:MSE:O	1:D:209:ASP:HB3	2.14	0.45
1:A:153:MSE:CE	1:A:202:ASN:ND2	2.80	0.45
1:A:75:VAL:CG2	1:A:76:LEU:N	2.80	0.45
1:A:233:GLU:OE1	1:A:287:LYS:HE3	2.17	0.45
1:D:29:MSE:HG3	1:D:31:LEU:H	1.82	0.45
1:B:116:PRO:HG2	1:B:119:ARG:NH2	2.32	0.45
1:C:241:ILE:HD11	1:C:275:MSE:HG3	1.98	0.45
1:A:73:GLN:HG2	1:A:85:GLN:CD	2.37	0.44
1:D:28:PRO:HD2	1:D:115:TRP:CZ3	2.52	0.44
1:A:313:ARG:NH1	1:A:313:ARG:HG2	2.32	0.44
1:B:36:ILE:HD12	1:B:48:LEU:HD12	1.99	0.44
1:B:129:PHE:CZ	1:B:173:PRO:HD2	2.52	0.44
1:D:58:LEU:O	1:D:62:LEU:HB2	2.16	0.44
1:D:29:MSE:HE1	1:D:51:VAL:CG1	2.31	0.44
1:B:209:ASP:O	1:B:210:TYR:HB3	2.18	0.44
1:C:296:ARG:HD3	1:D:208:MSE:HA	2.00	0.44
1:C:163:LEU:HA	1:C:163:LEU:HD12	1.86	0.44
1:D:86:ARG:HD2	1:D:86:ARG:HA	1.72	0.44
1:A:176:SER:HB3	1:A:179:ILE:HG12	2.00	0.44
1:A:36:ILE:HD12	1:A:48:LEU:HD12	2.00	0.44
1:C:8:LEU:HD13	1:C:9:MSE:HB3	1.99	0.44
1:C:266:THR:HG22	1:C:269:GLU:HB2	1.99	0.44
1:C:291:LEU:HD11	1:C:294:ARG:NH1	2.32	0.44
1:A:206:SER:HA	1:A:218:PHE:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:GLY:HA2	1:D:175:TYR:HB2	2.00	0.44
1:B:215:HIS:HD2	1:B:216:HIS:H	1.47	0.44
1:C:153:MSE:HG2	1:C:153:MSE:O	2.17	0.44
1:C:12:TYR:CE2	1:C:315:ARG:HB2	2.53	0.44
1:B:306:ASN:HD21	1:B:308:ALA:HB3	1.83	0.44
1:C:316:LYS:HG2	1:C:316:LYS:H	1.56	0.43
1:A:17:ARG:HH22	1:A:50:GLU:HA	1.82	0.43
1:B:86:ARG:CZ	1:B:192:GLN:HE22	2.30	0.43
1:B:286:LEU:CD2	1:B:291:LEU:HD22	2.46	0.43
1:B:163:LEU:HD13	1:B:170:VAL:HG11	2.00	0.43
1:A:42:ILE:HD13	1:A:247:PHE:HE2	1.83	0.43
1:A:266:THR:HG22	1:A:269:GLU:HB2	2.01	0.43
1:C:267:LYS:O	1:C:271:ILE:HG13	2.19	0.43
1:B:72:ARG:HG3	1:B:72:ARG:O	2.17	0.43
1:B:85:GLN:N	1:B:85:GLN:HE21	2.17	0.43
1:B:291:LEU:HD11	1:B:294:ARG:NH1	2.33	0.43
1:C:306:ASN:HD21	1:C:308:ALA:HB3	1.81	0.43
1:C:36:ILE:HD12	1:C:48:LEU:HD12	2.00	0.43
1:B:283:TRP:CZ2	1:B:287:LYS:HD2	2.53	0.43
1:D:207:GLY:HA2	1:D:210:TYR:CB	2.49	0.43
1:D:176:SER:HB3	1:D:179:ILE:HG12	1.99	0.43
1:C:96:SER:O	1:C:99:VAL:HG12	2.18	0.43
1:C:79:PHE:HB2	1:D:64:PHE:CD2	2.54	0.43
1:C:176:SER:HB3	1:C:179:ILE:HG12	2.01	0.43
1:D:291:LEU:HA	1:D:291:LEU:HD13	1.81	0.43
1:C:283:TRP:CZ2	1:C:287:LYS:HD2	2.53	0.43
1:B:47:SER:OG	1:B:49:GLU:HG2	2.19	0.43
1:B:28:PRO:HD2	1:B:115:TRP:CZ3	2.54	0.42
1:D:241:ILE:O	1:D:244:PHE:HB3	2.18	0.42
1:B:56:LEU:HA	1:B:56:LEU:HD23	1.86	0.42
1:B:121:VAL:HA	1:B:195:ILE:O	2.19	0.42
1:C:115:TRP:CB	1:C:116:PRO:CD	2.97	0.42
1:A:267:LYS:O	1:A:271:ILE:HG13	2.20	0.42
1:B:210:TYR:HA	1:B:213:ASP:OD1	2.19	0.42
1:D:283:TRP:CZ2	1:D:287:LYS:HD2	2.54	0.42
1:B:163:LEU:HD12	1:B:163:LEU:HA	1.88	0.42
1:D:73:GLN:CG	1:D:73:GLN:O	2.68	0.42
1:C:108:LEU:HD12	1:C:108:LEU:HA	1.94	0.42
1:C:128:GLY:HA2	1:C:175:TYR:HB2	2.01	0.42
1:B:29:MSE:HG3	1:B:31:LEU:H	1.83	0.42
1:C:126:THR:CG2	1:C:151:TYR:CE2	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ILE:HD13	1:C:247:PHE:HE2	1.84	0.42
1:C:121:VAL:HA	1:C:195:ILE:O	2.19	0.42
1:C:29:MSE:CE	1:C:51:VAL:HG11	2.35	0.42
1:B:75:VAL:CG2	1:B:76:LEU:N	2.82	0.42
1:B:71:ARG:HH11	1:B:71:ARG:HG3	1.84	0.42
1:C:28:PRO:HD2	1:C:115:TRP:CZ3	2.54	0.42
1:C:72:ARG:HA	1:D:70:LEU:HD21	2.01	0.42
1:B:264:LYS:NZ	1:C:139:ARG:HB3	2.35	0.42
1:A:126:THR:CG2	1:A:151:TYR:CE2	3.03	0.42
1:D:126:THR:CG2	1:D:151:TYR:CE2	3.03	0.42
1:A:11:PRO:CD	1:B:215:HIS:CB	2.96	0.42
1:D:237:GLN:NE2	1:D:275:MSE:HG2	2.35	0.42
1:A:304:SER:OG	1:A:310:GLU:HG2	2.20	0.42
1:B:70:LEU:HD13	1:B:70:LEU:HA	1.69	0.42
1:D:12:TYR:CE2	1:D:315:ARG:HB2	2.55	0.42
1:B:83:ASN:HB3	1:B:84:GLY:H	1.25	0.42
1:D:304:SER:OG	1:D:310:GLU:HG2	2.20	0.42
1:D:316:LYS:H	1:D:316:LYS:HG2	1.55	0.41
1:B:153:MSE:HG2	1:B:156:LEU:HB3	2.02	0.41
1:A:71:ARG:HH21	1:B:70:LEU:HD13	1.84	0.41
1:A:54:ILE:O	1:A:57:PRO:HD2	2.20	0.41
1:B:115:TRP:CB	1:B:116:PRO:CD	2.98	0.41
1:C:127:ASP:OD1	1:C:128:GLY:N	2.53	0.41
1:D:210:TYR:CB	1:D:211:PRO:CD	2.69	0.41
1:B:215:HIS:O	1:B:216:HIS:O	2.37	0.41
1:A:115:TRP:CB	1:A:116:PRO:CD	2.98	0.41
1:B:33:GLU:CG	1:B:48:LEU:HD13	2.50	0.41
1:D:36:ILE:HD12	1:D:48:LEU:HD12	2.01	0.41
1:D:133:ASN:O	1:D:137:LYS:HD3	2.21	0.41
1:B:17:ARG:HH22	1:B:50:GLU:HA	1.85	0.41
1:C:72:ARG:HG3	1:C:72:ARG:HH11	1.76	0.41
1:A:64:PHE:CE2	1:B:79:PHE:HA	2.52	0.41
1:B:127:ASP:OD1	1:B:128:GLY:N	2.53	0.41
1:D:47:SER:OG	1:D:49:GLU:HG2	2.20	0.41
1:A:291:LEU:HD11	1:A:294:ARG:NH1	2.36	0.41
1:A:24:ARG:HG3	1:A:25:ASP:N	2.33	0.41
1:B:128:GLY:HA2	1:B:175:TYR:HB2	2.03	0.41
1:D:223:VAL:HG21	3:D:736:HOH:O	2.20	0.41
1:B:85:GLN:CA	1:B:87:ILE:CD1	2.93	0.41
1:C:55:TYR:HE2	1:C:104:THR:HG23	1.84	0.41
1:C:129:PHE:CD2	1:C:155:ARG:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:LEU:HD12	1:D:204:LEU:HA	1.90	0.41
1:B:126:THR:HG23	1:B:151:TYR:CE2	2.55	0.41
1:B:115:TRP:CG	1:B:116:PRO:CD	3.04	0.41
1:C:116:PRO:HG2	1:C:119:ARG:NH2	2.35	0.41
1:B:40:LYS:HE3	1:B:46:LEU:H	1.86	0.41
1:B:97:VAL:HG12	1:B:201:LEU:HD21	2.02	0.41
1:B:133:ASN:O	1:B:137:LYS:HD3	2.21	0.41
1:A:56:LEU:HA	1:A:56:LEU:HD23	1.85	0.41
1:A:163:LEU:HD13	1:A:170:VAL:HG11	2.03	0.41
1:C:65:TYR:CD2	1:D:75:VAL:HG21	2.56	0.41
1:D:133:ASN:HA	1:D:133:ASN:HD22	1.74	0.41
1:C:72:ARG:HD2	1:C:76:LEU:HD22	2.02	0.40
1:A:71:ARG:HH21	1:B:70:LEU:CD1	2.34	0.40
1:C:163:LEU:HD13	1:C:170:VAL:HG11	2.03	0.40
1:D:70:LEU:HD12	1:D:70:LEU:HA	1.86	0.40
1:A:163:LEU:HA	1:A:163:LEU:HD12	1.86	0.40
1:C:17:ARG:HH22	1:C:50:GLU:HA	1.85	0.40
1:A:12:TYR:CE2	1:A:315:ARG:HB2	2.56	0.40
1:B:291:LEU:HD13	1:B:291:LEU:HA	1.83	0.40
1:D:126:THR:HG23	1:D:151:TYR:CE2	2.56	0.40
1:C:306:ASN:HD22	1:C:308:ALA:HB3	1.86	0.40
1:A:47:SER:OG	1:A:49:GLU:HG2	2.22	0.40
1:D:17:ARG:HH22	1:D:50:GLU:HA	1.85	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	309/316 (98%)	284 (92%)	18 (6%)	7 (2%)	8	12
1	B	303/316 (96%)	279 (92%)	17 (6%)	7 (2%)	8	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	303/316 (96%)	278 (92%)	20 (7%)	5 (2%)	11	19
1	D	297/316 (94%)	273 (92%)	15 (5%)	9 (3%)	5	7
All	All	1212/1264 (96%)	1114 (92%)	70 (6%)	28 (2%)	8	12

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	86	ARG
1	A	168	PRO
1	B	69	ASN
1	B	168	PRO
1	B	214	PRO
1	C	168	PRO
1	D	69	ASN
1	D	115	TRP
1	D	168	PRO
1	D	209	ASP
1	D	210	TYR
1	A	115	TRP
1	B	115	TRP
1	B	216	HIS
1	C	115	TRP
1	A	120	ARG
1	B	120	ARG
1	C	87	ILE
1	D	120	ARG
1	A	121	VAL
1	A	210	TYR
1	B	121	VAL
1	C	121	VAL
1	D	121	VAL
1	C	120	ARG
1	D	70	LEU
1	D	79	PHE

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	280/278 (101%)	234 (84%)	46 (16%)	3	5
1	B	276/278 (99%)	230 (83%)	46 (17%)	3	5
1	C	276/278 (99%)	227 (82%)	49 (18%)	2	3
1	D	273/278 (98%)	222 (81%)	51 (19%)	2	3
All	All	1105/1112 (99%)	913 (83%)	192 (17%)	2	4

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	THR
1	A	10	THR
1	A	17	ARG
1	A	24	ARG
1	A	27	VAL
1	A	29	MSE
1	A	38	ARG
1	A	49	GLU
1	A	62	LEU
1	A	68	SER
1	A	69	ASN
1	A	70	LEU
1	A	78	GLN
1	A	83	ASN
1	A	85	GLN
1	A	86	ARG
1	A	90	ILE
1	A	93	ILE
1	A	101	LYS
1	A	107	VAL
1	A	114	ARG
1	A	115	TRP
1	A	120	ARG
1	A	126	THR
1	A	137	LYS
1	A	145	LYS
1	A	182	VAL
1	A	191	VAL
1	A	199	GLU

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Mol	Chain	Res	Type
1	A	204	LEU
1	A	248	ARG
1	A	264	LYS
1	A	272	LYS
1	A	276	THR
1	A	284	LEU
1	A	286	LEU
1	A	287	LYS
1	A	289	ASN
1	A	291	LEU
1	A	296	ARG
1	A	298	SER
1	A	304	SER
1	A	306	ASN
1	A	313	ARG
1	A	316	LYS
1	B	10	THR
1	B	17	ARG
1	B	24	ARG
1	B	27	VAL
1	B	29	MSE
1	B	38	ARG
1	B	48	LEU
1	B	49	GLU
1	B	62	LEU
1	B	70	LEU
1	B	72	ARG
1	B	76	LEU
1	B	82	THR
1	B	83	ASN
1	B	86	ARG
1	B	90	ILE
1	B	93	ILE
1	B	101	LYS
1	B	107	VAL
1	B	114	ARG
1	B	115	TRP
1	B	120	ARG
1	B	126	THR
1	B	137	LYS
1	B	145	LYS
1	B	182	VAL

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Mol	Chain	Res	Type
1	B	191	VAL
1	B	199	GLU
1	B	204	LEU
1	B	206	SER
1	B	215	HIS
1	B	248	ARG
1	B	264	LYS
1	B	272	LYS
1	B	276	THR
1	B	284	LEU
1	B	286	LEU
1	B	287	LYS
1	B	289	ASN
1	B	291	LEU
1	B	296	ARG
1	B	298	SER
1	B	304	SER
1	B	306	ASN
1	B	313	ARG
1	B	316	LYS
1	C	7	THR
1	C	8	LEU
1	C	10	THR
1	C	17	ARG
1	C	24	ARG
1	C	27	VAL
1	C	29	MSE
1	C	38	ARG
1	C	48	LEU
1	C	49	GLU
1	C	62	LEU
1	C	67	SER
1	C	71	ARG
1	C	72	ARG
1	C	76	LEU
1	C	78	GLN
1	C	80	LEU
1	C	85	GLN
1	C	86	ARG
1	C	90	ILE
1	C	93	ILE
1	C	101	LYS

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Mol	Chain	Res	Type
1	C	107	VAL
1	C	114	ARG
1	C	115	TRP
1	C	120	ARG
1	C	126	THR
1	C	137	LYS
1	C	145	LYS
1	C	182	VAL
1	C	191	VAL
1	C	199	GLU
1	C	204	LEU
1	C	215	HIS
1	C	248	ARG
1	C	264	LYS
1	C	272	LYS
1	C	276	THR
1	C	284	LEU
1	C	286	LEU
1	C	287	LYS
1	C	289	ASN
1	C	291	LEU
1	C	296	ARG
1	C	298	SER
1	C	304	SER
1	C	306	ASN
1	C	313	ARG
1	C	316	LYS
1	D	8	LEU
1	D	9	MSE
1	D	17	ARG
1	D	24	ARG
1	D	27	VAL
1	D	29	MSE
1	D	38	ARG
1	D	48	LEU
1	D	49	GLU
1	D	62	LEU
1	D	68	SER
1	D	70	LEU
1	D	71	ARG
1	D	72	ARG
1	D	73	GLN

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Mol	Chain	Res	Type
1	D	76	LEU
1	D	77	GLU
1	D	78	GLN
1	D	80	LEU
1	D	82	THR
1	D	86	ARG
1	D	90	ILE
1	D	93	ILE
1	D	101	LYS
1	D	107	VAL
1	D	114	ARG
1	D	115	TRP
1	D	120	ARG
1	D	126	THR
1	D	137	LYS
1	D	145	LYS
1	D	182	VAL
1	D	191	VAL
1	D	199	GLU
1	D	204	LEU
1	D	209	ASP
1	D	210	TYR
1	D	248	ARG
1	D	264	LYS
1	D	272	LYS
1	D	276	THR
1	D	284	LEU
1	D	286	LEU
1	D	287	LYS
1	D	289	ASN
1	D	291	LEU
1	D	296	ARG
1	D	304	SER
1	D	306	ASN
1	D	313	ARG
1	D	316	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	69	ASN

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Mol	Chain	Res	Type
1	A	73	GLN
1	A	85	GLN
1	A	133	ASN
1	A	260	HIS
1	A	306	ASN
1	B	14	GLN
1	B	78	GLN
1	B	85	GLN
1	B	133	ASN
1	B	192	GLN
1	B	215	HIS
1	B	216	HIS
1	B	260	HIS
1	B	306	ASN
1	C	14	GLN
1	C	73	GLN
1	C	133	ASN
1	C	192	GLN
1	C	215	HIS
1	C	260	HIS
1	C	306	ASN
1	D	14	GLN
1	D	73	GLN
1	D	118	HIS
1	D	133	ASN
1	D	216	HIS
1	D	260	HIS
1	D	306	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)

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	COA	A	401	-	40,50,50	3.02	6 (15%)	50,75,75	2.29	16 (32%)
2	COA	B	404	-	40,50,50	3.00	5 (12%)	50,75,75	2.31	16 (32%)
2	COA	C	402	-	40,50,50	2.99	6 (15%)	50,75,75	2.91	17 (34%)
2	COA	D	403	-	40,50,50	2.99	5 (12%)	50,75,75	2.31	18 (36%)

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	COA	A	401	-	-	0/44/64/64	0/3/3/3
2	COA	B	404	-	-	0/44/64/64	0/3/3/3
2	COA	C	402	-	-	0/44/64/64	0/3/3/3
2	COA	D	403	-	-	0/44/64/64	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	404	COA	O9P-C9P	-11.94	1.00	1.23
2	A	401	COA	O9P-C9P	-11.80	1.00	1.23
2	C	402	COA	O9P-C9P	-11.79	1.00	1.23
2	D	403	COA	O9P-C9P	-11.63	1.00	1.23
2	C	402	COA	P3B-O9A	-2.29	1.46	1.54
2	D	403	COA	P3B-O9A	-2.25	1.46	1.54
2	B	404	COA	P3B-O9A	-2.23	1.46	1.54
2	A	401	COA	P3B-O9A	-2.22	1.46	1.54
2	A	401	COA	C7P-C6P	2.02	1.57	1.51
2	C	402	COA	C4A-N3A	2.25	1.38	1.35
2	A	401	COA	C4A-N3A	2.28	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	404	COA	C7P-C6P	2.40	1.59	1.51
2	D	403	COA	C4A-N3A	2.43	1.39	1.35
2	C	402	COA	OAP-CAP	2.67	1.47	1.42
2	A	401	COA	C7P-N8P	2.73	1.52	1.46
2	C	402	COA	C7P-N8P	2.87	1.52	1.46
2	D	403	COA	C7P-N8P	2.90	1.53	1.46
2	B	404	COA	C7P-N8P	3.02	1.53	1.46
2	C	402	COA	C9P-N8P	12.47	1.59	1.33
2	B	404	COA	C9P-N8P	12.66	1.60	1.33
2	D	403	COA	C9P-N8P	12.91	1.60	1.33
2	A	401	COA	C9P-N8P	13.00	1.60	1.33

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	COA	CAP-C9P-N8P	-6.29	102.54	116.47
2	D	403	COA	CAP-C9P-N8P	-6.23	102.67	116.47
2	B	404	COA	CAP-C9P-N8P	-6.11	102.94	116.47
2	C	402	COA	CAP-C9P-N8P	-5.98	103.22	116.47
2	C	402	COA	C6P-C5P-N4P	-4.59	108.48	116.46
2	B	404	COA	C6P-C5P-N4P	-4.54	108.57	116.46
2	A	401	COA	C6P-C5P-N4P	-4.40	108.82	116.46
2	D	403	COA	C6P-C5P-N4P	-4.26	109.05	116.46
2	A	401	COA	C2P-C3P-N4P	-4.10	104.27	112.37
2	D	403	COA	C2P-C3P-N4P	-4.07	104.34	112.37
2	C	402	COA	O9P-C9P-N8P	-4.03	114.99	123.08
2	C	402	COA	C2P-C3P-N4P	-3.98	104.51	112.37
2	B	404	COA	C2P-C3P-N4P	-3.90	104.68	112.37
2	B	404	COA	O9P-C9P-N8P	-3.86	115.33	123.08
2	D	403	COA	O9P-C9P-N8P	-3.74	115.57	123.08
2	A	401	COA	O9P-C9P-N8P	-3.52	116.02	123.08
2	B	404	COA	OAP-CAP-C9P	-3.35	102.68	110.38
2	D	403	COA	CDP-CBP-CCP	-3.30	104.22	108.50
2	A	401	COA	OAP-CAP-C9P	-3.30	102.82	110.38
2	D	403	COA	OAP-CAP-C9P	-3.23	102.98	110.38
2	A	401	COA	CDP-CBP-CCP	-3.17	104.40	108.50
2	B	404	COA	CDP-CBP-CCP	-3.11	104.47	108.50
2	C	402	COA	CEP-CBP-CDP	-2.87	103.52	109.28
2	C	402	COA	CDP-CBP-CCP	-2.84	104.83	108.50
2	A	401	COA	CEP-CBP-CDP	-2.79	103.67	109.28
2	B	404	COA	CEP-CBP-CDP	-2.68	103.89	109.28
2	D	403	COA	CEP-CBP-CDP	-2.47	104.31	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	403	COA	P2A-O3A-P1A	-2.45	125.84	132.73
2	C	402	COA	P2A-O3A-P1A	-2.36	126.09	132.73
2	A	401	COA	C1B-N9A-C4A	-2.32	123.44	126.94
2	C	402	COA	C1B-N9A-C4A	-2.23	123.58	126.94
2	A	401	COA	P2A-O3A-P1A	-2.22	126.51	132.73
2	B	404	COA	P2A-O3A-P1A	-2.18	126.61	132.73
2	D	403	COA	N3A-C2A-N1A	-2.07	127.31	128.89
2	D	403	COA	C1B-N9A-C4A	-2.06	123.83	126.94
2	B	404	COA	C1B-N9A-C4A	-2.02	123.89	126.94
2	D	403	COA	C4A-C5A-N7A	2.03	111.35	109.48
2	C	402	COA	CEP-CBP-CAP	2.07	113.13	109.34
2	D	403	COA	O3A-P1A-O5B	2.15	108.63	102.94
2	B	404	COA	C3P-N4P-C5P	2.15	127.02	122.79
2	A	401	COA	O5P-C5P-N4P	2.18	127.27	122.94
2	A	401	COA	O3A-P1A-O5B	2.22	108.81	102.94
2	B	404	COA	O3A-P1A-O5B	2.25	108.90	102.94
2	A	401	COA	C3P-N4P-C5P	2.25	127.22	122.79
2	B	404	COA	O5P-C5P-N4P	2.32	127.53	122.94
2	C	402	COA	P3B-O3B-C3B	2.34	127.17	121.56
2	D	403	COA	O5P-C5P-N4P	2.37	127.64	122.94
2	C	402	COA	C3P-N4P-C5P	2.39	127.50	122.79
2	C	402	COA	O5P-C5P-N4P	2.40	127.70	122.94
2	C	402	COA	O3A-P1A-O5B	2.47	109.49	102.94
2	D	403	COA	C3P-N4P-C5P	2.50	127.71	122.79
2	B	404	COA	O9A-P3B-O7A	2.58	118.88	110.58
2	A	401	COA	P3B-O3B-C3B	2.65	127.91	121.56
2	C	402	COA	O9A-P3B-O7A	2.77	119.48	110.58
2	D	403	COA	O9A-P3B-O7A	2.77	119.49	110.58
2	A	401	COA	O9A-P3B-O7A	2.80	119.60	110.58
2	B	404	COA	P3B-O3B-C3B	2.89	128.48	121.56
2	D	403	COA	P3B-O3B-C3B	2.98	128.71	121.56
2	A	401	COA	C2B-C1B-N9A	4.97	121.88	114.29
2	D	403	COA	C2B-C1B-N9A	5.33	122.44	114.29
2	C	402	COA	C2B-C1B-N9A	5.51	122.72	114.29
2	B	404	COA	C2B-C1B-N9A	5.65	122.92	114.29
2	A	401	COA	O3A-P2A-O6A	6.58	120.40	102.94
2	C	402	COA	O3A-P2A-O6A	6.65	120.57	102.94
2	D	403	COA	O3A-P2A-O6A	6.70	120.70	102.94
2	B	404	COA	O3A-P2A-O6A	6.79	120.95	102.94
2	C	402	COA	OAP-CAP-C9P	12.84	139.84	110.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	305/316 (96%)	0.15	15 (4%)	33	38	14, 31, 54, 78	0
1	B	301/316 (95%)	0.03	10 (3%)	50	55	10, 28, 53, 94	0
1	C	301/316 (95%)	0.05	8 (2%)	58	62	15, 30, 51, 75	0
1	D	297/316 (93%)	-0.01	5 (1%)	73	76	15, 29, 48, 82	0
All	All	1204/1264 (95%)	0.06	38 (3%)	51	56	10, 29, 52, 94	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	84	GLY	6.4
1	A	210	TYR	5.1
1	B	82	THR	3.8
1	A	85	GLN	3.5
1	A	168	PRO	3.5
1	C	115	TRP	3.3
1	B	86	ARG	3.2
1	B	83	ASN	3.1
1	B	85	GLN	3.1
1	C	168	PRO	3.1
1	A	86	ARG	3.1
1	A	213	ASP	3.0
1	A	7	THR	3.0
1	D	115	TRP	3.0
1	B	215	HIS	2.9
1	D	86	ARG	2.8
1	D	140	GLY	2.7
1	D	210	TYR	2.7
1	A	115	TRP	2.7
1	B	115	TRP	2.7
1	A	8	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	8	LEU	2.7
1	B	70	LEU	2.6
1	C	167	VAL	2.6
1	A	6	GLN	2.4
1	B	168	PRO	2.4
1	A	185	ASP	2.3
1	A	82	THR	2.3
1	C	83	ASN	2.3
1	C	215	HIS	2.3
1	B	81	GLY	2.3
1	A	212	HIS	2.2
1	A	184	PRO	2.1
1	A	154	HIS	2.1
1	A	266	THR	2.1
1	C	185	ASP	2.1
1	D	209	ASP	2.1
1	C	184	PRO	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
2	COA	D	403	48/48	0.94	0.17	1.14	23,34,41,48	0
2	COA	B	404	48/48	0.95	0.16	0.96	22,29,38,42	0
2	COA	C	402	48/48	0.96	0.16	0.94	18,32,40,46	0
2	COA	A	401	48/48	0.95	0.15	0.36	25,35,39,44	0

6.5 Other polymers (i)

There are no such residues in this entry.