W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 12:35 am GMT

PDB ID	:	2I7P
Title	:	Crystal structure of human PANK3 in complex with AcCoA
Authors	:	Hong, B.S.; Wang, L.; Shen, L.; Tempel, W.; Loppnau, P.; Finerty, P.; Arrowsmith, C.H.; Edwards, A.M.; Sundstrom, M.; Weigelt, J.; Bochkarev, A.; Park, H.W.; Structural Genomics Consortium (SGC)
Deposited on	:	2006-08-31
Resolution	:	2.05 Å(reported)

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

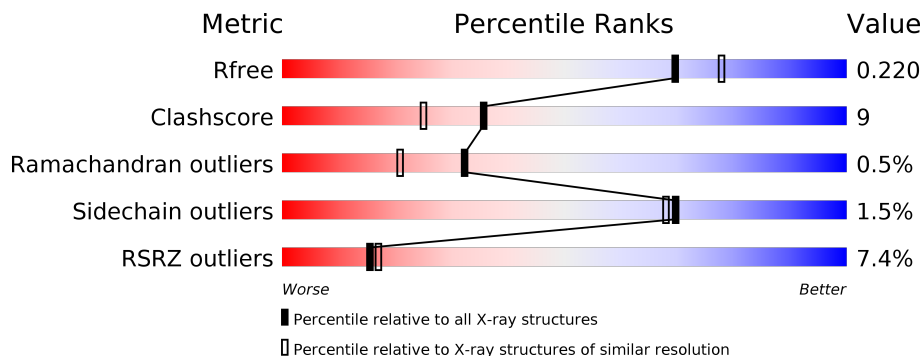|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.05 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	Percentile Ranks	Value
Rfree		0.220
Clashscore		9
Ramachandran outliers		0.5%
Sidechain outliers		1.5%
RSRZ outliers		7.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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	362	6% / 76% / 21% / ••
1	B	362	7% / 81% / 16% / ••
1	C	362	7% / 78% / 17% / • •
1	D	362	9% / 80% / 15% / ••

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11796 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.
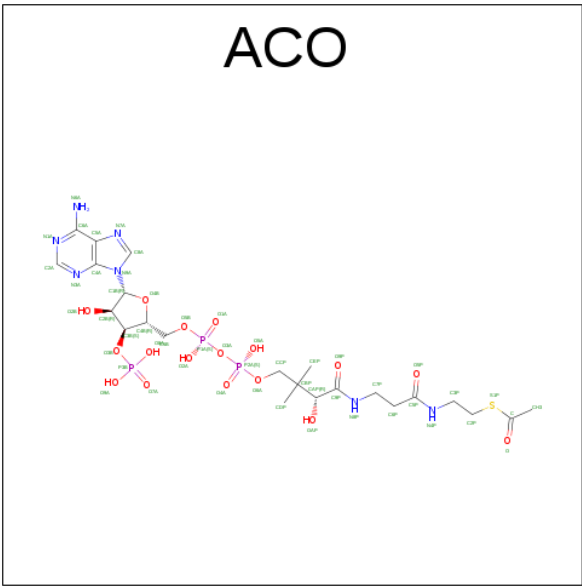
- Molecule 1 is a protein called Pantothenate kinase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2759	1760	464	521	14			
1	B	354	Total	C	N	O	S	0	0	0
			2765	1763	465	523	14			
1	C	348	Total	C	N	O	S	0	0	0
			2719	1735	456	514	14			
1	D	348	Total	C	N	O	S	0	0	0
			2722	1738	456	514	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	VAL	-	CLONING ARTIFACT	UNP Q9H999
A	8	PRO	-	CLONING ARTIFACT	UNP Q9H999
A	9	ARG	-	CLONING ARTIFACT	UNP Q9H999
A	10	GLY	-	CLONING ARTIFACT	UNP Q9H999
A	11	SER	-	CLONING ARTIFACT	UNP Q9H999
B	7	VAL	-	CLONING ARTIFACT	UNP Q9H999
B	8	PRO	-	CLONING ARTIFACT	UNP Q9H999
B	9	ARG	-	CLONING ARTIFACT	UNP Q9H999
B	10	GLY	-	CLONING ARTIFACT	UNP Q9H999
B	11	SER	-	CLONING ARTIFACT	UNP Q9H999
C	7	VAL	-	CLONING ARTIFACT	UNP Q9H999
C	8	PRO	-	CLONING ARTIFACT	UNP Q9H999
C	9	ARG	-	CLONING ARTIFACT	UNP Q9H999
C	10	GLY	-	CLONING ARTIFACT	UNP Q9H999
C	11	SER	-	CLONING ARTIFACT	UNP Q9H999
D	7	VAL	-	CLONING ARTIFACT	UNP Q9H999
D	8	PRO	-	CLONING ARTIFACT	UNP Q9H999
D	9	ARG	-	CLONING ARTIFACT	UNP Q9H999
D	10	GLY	-	CLONING ARTIFACT	UNP Q9H999
D	11	SER	-	CLONING ARTIFACT	UNP Q9H999

- 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 29	C 13	N 2	O 11	P 2	S 1	0	0
2	B	1	Total 29	C 13	N 2	O 11	P 2	S 1	0	0
2	C	1	Total 29	C 13	N 2	O 11	P 2	S 1	0	0
2	D	1	Total 29	C 13	N 2	O 11	P 2	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	206	Total 206	O 206	0	0
3	B	155	Total 155	O 155	0	0
3	C	164	Total 164	O 164	0	0
3	D	190	Total 190	O 190	0	0

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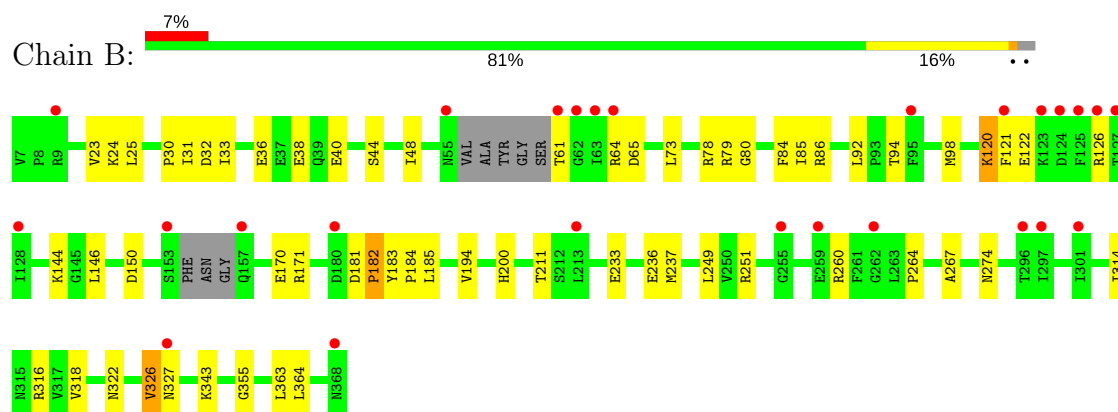y criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present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

• Molecule 1: Pantothenate kinase 3

Chain A:

• Molecule 1: Pantothenate kinase 3

Chain B:

• Molecule 1: Pantothenate kinase 3

Chain C:

V284 S285 K286 I297 C308 N311 R316 N322 R325 V326 N327 L363 G365 LEU PRO ASN

• Molecule 1: Pantothenate kinase 3

Chain D:

9%

80% 15%

VAL PRO ARG GLY SER P12 W13 D17 K24 I31 D32 I33 T34 A35 E36 E37 E38 E41 V42 L45 N55 VAL ALA TYR GLY SER THR G62 I63 D72 F76 G77 R78 R79 G80 N81 T94 M98 G99 F104 S105 T106 L107 Q108 T109 V110 L111 C112

Y119 K120 K123 R126 T127 I128 G129 N130 L131 H132 L133 H134 L146 F154 Q157 N165 R171 L179 Y183 I190 V194 K206 R207 V208 T211 S212 L213 G214 E229 E233 M237 G241 D242 Q245 R251 D257 Y258 E259 L263

K278 E279 E282 S283 V284 S285 K286 E287 I297 I301 G302 S303 R306 N311 R316 N327 W341 L363 L364 G365 LEU PRO ASN

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.73Å 180.17Å 77.73Å 90.00° 95.68° 90.00°	Depositor
Resolution (Å)	29.34 – 2.05 29.34 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.34-2.05) 98.6 (29.34-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.04Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.253 0.213 , 0.220	Depositor DCC
R_{free} test set	4782 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11796	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 3.94% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5　Model quality ⓘ

5.1　Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.35	0/2812	0.56	0/3793
1	B	0.34	0/2818	0.55	0/3801
1	C	0.34	0/2772	0.55	0/3738
1	D	0.35	0/2775	0.56	0/3742
All	All	0.34	0/11177	0.56	0/15074

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2　Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2759	0	2744	72	0
1	B	2765	0	2749	45	0
1	C	2719	0	2691	52	0
1	D	2722	0	2701	43	0
2	A	29	0	22	0	0
2	B	29	0	22	0	0
2	C	29	0	22	0	0
2	D	29	0	23	0	0
3	A	206	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	155	0	0	1	0
3	C	164	0	0	2	0
3	D	190	0	0	6	0
All	All	11796	0	10974	203	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 9.

All (203) 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:A:327:ASN:HD22	1:A:329:LEU:HB3	1.29	0.95
1:A:327:ASN:ND2	1:A:330:SER:H	1.67	0.92
1:D:31:ILE:HG12	1:D:80:GLY:HA2	1.54	0.86
1:C:228:CYS:HB3	1:C:237:MET:CE	2.09	0.82
1:D:110:VAL:HG12	1:D:132:HIS:HB2	1.64	0.80
1:A:311:ASN:HD21	1:C:311:ASN:HB2	1.48	0.78
1:B:30:PRO:HB2	1:B:33:ILE:HD11	1.67	0.77
1:C:228:CYS:HB3	1:C:237:MET:HE1	1.66	0.76
1:D:99:GLY:HA3	1:D:107:LEU:HD12	1.70	0.72
1:C:182:PRO:HA	1:C:316:ARG:HH11	1.55	0.71
1:A:327:ASN:HD21	1:A:330:SER:H	1.36	0.71
1:C:226:THR:HA	1:C:286:LYS:HD2	1.71	0.70
1:A:180:ASP:O	1:A:182:PRO:HD3	1.91	0.70
1:A:124:ASP:O	1:A:127:THR:HG22	1.92	0.69
1:A:327:ASN:ND2	1:A:330:SER:N	2.39	0.68
1:A:327:ASN:HD21	1:A:330:SER:N	1.93	0.66
1:A:327:ASN:ND2	1:A:329:LEU:HB3	2.08	0.66
1:B:120:LYS:HB2	1:B:120:LYS:NZ	2.12	0.65
1:A:90:GLN:HG3	3:A:1718:HOH:O	1.95	0.65
1:D:110:VAL:HG12	1:D:132:HIS:CB	2.27	0.64
1:C:228:CYS:HB3	1:C:237:MET:HE3	1.79	0.64
1:C:104:PHE:O	1:C:108:GLN:HG2	1.99	0.63
1:A:31:ILE:HG13	1:A:80:GLY:HA2	1.81	0.63
1:A:278:LYS:HG2	1:A:281:ARG:NH2	2.14	0.62
1:D:129:GLY:HA3	3:D:2063:HOH:O	2.00	0.62
1:D:311:ASN:HB3	3:D:2081:HOH:O	2.00	0.62
1:A:171:ARG:HD2	3:A:1743:HOH:O	2.00	0.61
1:A:105:SER:HA	1:A:108:GLN:HG3	1.83	0.61
1:A:236:GLU:HG3	1:A:240:LYS:HE2	1.83	0.61
1:A:194:VAL:HB	1:A:211:THR:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:VAL:HB	1:C:211:THR:HG22	1.82	0.60
1:D:38:GLU:OE2	1:D:78:ARG:NH1	2.34	0.60
1:C:179:LEU:HG	1:C:182:PRO:HB3	1.83	0.60
1:B:30:PRO:HB2	1:B:33:ILE:CD1	2.32	0.59
1:A:279:GLU:OE1	1:A:279:GLU:N	2.28	0.59
1:C:39:GLN:O	1:C:43:GLU:HG3	2.03	0.59
1:B:181:ASP:O	1:B:316:ARG:NH1	2.36	0.59
1:B:343:LYS:HE2	3:B:1817:HOH:O	2.01	0.59
1:B:24:LYS:HD3	1:B:355:GLY:O	2.03	0.58
1:A:326:VAL:O	1:A:326:VAL:HG12	2.03	0.58
1:D:33:ILE:HD11	1:D:42:VAL:HG21	1.84	0.58
1:D:179:LEU:CD1	1:D:316:ARG:HD2	2.34	0.58
1:C:200:HIS:HB2	1:C:204:ASN:ND2	2.18	0.57
1:A:235:LEU:HD13	1:A:327:ASN:HB3	1.86	0.57
1:A:246:ALA:HA	1:A:275:MET:CE	2.34	0.57
1:D:257:ASP:HB3	3:D:1964:HOH:O	2.04	0.57
1:C:208:VAL:HG21	1:C:308:CYS:SG	2.45	0.57
1:A:24:LYS:HE3	1:A:24:LYS:N	2.20	0.56
1:B:144:LYS:HG2	1:B:364:LEU:HD12	1.88	0.56
1:D:31:ILE:HD11	1:D:81:ASN:ND2	2.21	0.56
1:D:94:THR:O	1:D:98:MET:HG3	2.05	0.55
1:D:183:TYR:C	1:D:316:ARG:HH21	2.10	0.55
1:C:168:GLU:OE2	1:C:171:ARG:HD2	2.07	0.55
1:C:99:GLY:HA3	1:C:107:LEU:HD12	1.87	0.55
1:A:185:LEU:HD11	1:A:318:VAL:HG23	1.89	0.54
1:A:36:GLU:O	1:A:40:GLU:HG3	2.08	0.54
1:B:36:GLU:O	1:B:40:GLU:HG3	2.07	0.54
1:B:194:VAL:HB	1:B:211:THR:HG22	1.90	0.54
1:A:279:GLU:CD	1:A:279:GLU:H	2.12	0.53
1:B:31:ILE:HB	1:B:80:GLY:HA2	1.89	0.53
1:C:181:ASP:O	1:C:316:ARG:NH1	2.41	0.53
1:C:322:ASN:HA	1:C:325:ARG:HD2	1.90	0.53
1:C:9:ARG:HG3	1:C:9:ARG:HH11	1.73	0.53
1:D:179:LEU:HD12	1:D:316:ARG:HD2	1.91	0.53
1:D:41:GLU:O	1:D:45:LEU:HG	2.09	0.52
1:A:246:ALA:HA	1:A:275:MET:HE3	1.92	0.52
1:A:25:LEU:HD23	1:A:85:ILE:HD11	1.90	0.52
1:A:194:VAL:HB	1:A:211:THR:CG2	2.40	0.51
1:B:65:ASP:HB3	1:B:84:PHE:O	2.10	0.51
1:D:206:LYS:HE3	1:D:208:VAL:HG12	1.91	0.51
1:A:322:ASN:HB3	1:A:325:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:VAL:HG12	1:B:327:ASN:N	2.25	0.51
1:D:183:TYR:C	1:D:316:ARG:NH2	2.63	0.51
1:B:122:GLU:O	1:B:126:ARG:HG3	2.11	0.51
1:B:120:LYS:HB2	1:B:120:LYS:HZ3	1.76	0.51
1:B:25:LEU:HD23	1:B:85:ILE:HD11	1.92	0.51
1:D:242:ASP:OD2	1:D:245:GLN:HG2	2.11	0.51
1:A:184:PRO:HB2	1:A:314:ILE:HG12	1.93	0.51
1:A:139:LEU:HD12	1:C:261:PHE:CE1	2.46	0.51
1:C:94:THR:O	1:C:98:MET:HG3	2.11	0.51
1:A:303:SER:HB2	1:A:341:TRP:CE2	2.46	0.50
1:C:363:LEU:HD23	1:C:363:LEU:O	2.11	0.50
1:D:13:TRP:CH2	1:D:76:PHE:HB2	2.47	0.50
1:B:194:VAL:HB	1:B:211:THR:CG2	2.42	0.50
1:C:122:GLU:OE2	1:C:133:LEU:HB3	2.12	0.50
1:D:327:ASN:HB3	3:D:2053:HOH:O	2.12	0.50
1:A:39:GLN:HG2	1:B:171:ARG:CZ	2.41	0.50
1:C:197:LEU:HD23	1:C:207:ARG:HA	1.94	0.50
1:A:258:TYR:HB3	1:A:263:LEU:HB2	1.92	0.49
1:D:306:ARG:C	1:D:306:ARG:HD2	2.33	0.49
1:D:306:ARG:HD2	1:D:306:ARG:O	2.12	0.49
1:B:249:LEU:HB2	1:B:251:ARG:HG2	1.93	0.49
1:B:94:THR:O	1:B:98:MET:HG3	2.13	0.49
1:B:38:GLU:CD	1:B:78:ARG:HH12	2.16	0.49
1:C:233:GLU:HG2	1:C:237:MET:HE2	1.94	0.49
1:A:62:GLY:HA3	3:A:1742:HOH:O	2.13	0.49
1:A:275:MET:HG3	1:C:224:LEU:HD11	1.96	0.48
1:B:183:TYR:HB3	1:B:200:HIS:O	2.14	0.48
1:A:192:SER:HA	1:A:216:GLY:H	1.79	0.48
1:B:61:THR:HA	1:B:64:ARG:HD2	1.95	0.48
1:C:33:ILE:HD11	1:C:42:VAL:HG21	1.94	0.48
1:A:49:ARG:HG3	1:A:85:ILE:HG21	1.96	0.48
1:C:99:GLY:HA3	1:C:107:LEU:CD1	2.43	0.48
1:B:126:ARG:HG2	1:B:126:ARG:HH11	1.78	0.47
1:D:41:GLU:HG3	1:D:104:PHE:CE1	2.49	0.47
1:D:111:LEU:HB2	1:D:131:LEU:HD11	1.95	0.47
1:C:109:THR:HG22	1:C:110:VAL:HG13	1.96	0.47
1:A:170:GLU:HG2	3:A:1667:HOH:O	2.14	0.47
1:A:363:LEU:HD23	1:A:363:LEU:C	2.35	0.47
1:C:322:ASN:HA	1:C:325:ARG:CD	2.44	0.47
1:A:175:MET:HA	1:A:175:MET:HE2	1.96	0.47
1:A:200:HIS:HE1	3:A:1666:HOH:O	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ASN:HB2	3:A:1766:HOH:O	2.14	0.47
1:D:99:GLY:HA3	1:D:107:LEU:CD1	2.44	0.47
1:D:233:GLU:O	1:D:237:MET:HG3	2.15	0.47
1:D:363:LEU:HD23	1:D:363:LEU:C	2.35	0.46
1:D:157:GLN:HA	1:D:157:GLN:OE1	2.14	0.46
1:B:92:LEU:HD23	1:B:121:PHE:CD1	2.51	0.46
1:B:170:GLU:HA	1:B:170:GLU:OE1	2.16	0.46
1:A:138:GLU:HG3	3:A:1799:HOH:O	2.15	0.46
1:A:322:ASN:HA	1:A:325:ARG:HD2	1.97	0.46
1:C:182:PRO:HA	1:C:316:ARG:NH1	2.28	0.46
1:D:146:LEU:HD23	1:D:146:LEU:C	2.36	0.46
1:A:92:LEU:HD23	1:A:121:PHE:CD1	2.51	0.46
1:C:322:ASN:HB3	1:C:325:ARG:NH1	2.31	0.46
1:D:110:VAL:HG23	3:D:1991:HOH:O	2.15	0.46
1:A:131:LEU:HD23	3:A:1683:HOH:O	2.16	0.45
1:D:286:LYS:HG3	3:D:1968:HOH:O	2.15	0.45
1:A:65:ASP:HB3	1:A:84:PHE:O	2.15	0.45
1:B:150:ASP:OD1	1:B:182:PRO:HG3	2.16	0.45
1:C:286:LYS:HG2	3:C:1920:HOH:O	2.15	0.45
1:A:182:PRO:HG2	1:A:183:TYR:CD1	2.52	0.45
1:D:12:PRO:HD2	1:D:104:PHE:HB3	1.97	0.45
1:A:185:LEU:HD11	1:A:318:VAL:CG2	2.47	0.45
1:A:23:VAL:O	1:A:86:ARG:HA	2.16	0.44
1:D:363:LEU:HD23	1:D:363:LEU:O	2.17	0.44
1:D:17:ASP:HB3	1:D:24:LYS:HB2	1.99	0.44
1:A:182:PRO:O	1:A:185:LEU:HB2	2.18	0.44
1:A:363:LEU:O	1:A:363:LEU:HD23	2.18	0.44
1:B:184:PRO:HB2	1:B:314:ILE:HG12	2.00	0.44
1:A:127:THR:HG23	1:A:128:ILE:HG23	1.99	0.44
1:C:278:LYS:O	1:C:282:GLU:HG3	2.18	0.44
1:D:303:SER:HB2	1:D:341:TRP:CE2	2.51	0.44
1:A:99:GLY:HA3	1:A:107:LEU:HD12	1.99	0.43
1:C:281:ARG:O	1:C:284:VAL:HG12	2.17	0.43
1:C:235:LEU:HB3	1:C:327:ASN:HD22	1.82	0.43
1:C:9:ARG:NH1	1:C:9:ARG:HG3	2.33	0.43
1:D:258:TYR:HB3	1:D:263:LEU:HB2	2.00	0.43
1:A:24:LYS:HE3	1:A:24:LYS:H	1.83	0.43
1:A:39:GLN:CG	1:B:171:ARG:CZ	2.96	0.43
1:C:130:ASN:HD22	1:C:131:LEU:N	2.17	0.43
1:C:73:LEU:HD23	1:C:73:LEU:O	2.18	0.43
1:A:92:LEU:HG	1:A:121:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:HIS:HB2	1:C:204:ASN:HD22	1.81	0.43
1:A:322:ASN:HA	1:A:325:ARG:CD	2.49	0.42
1:B:146:LEU:HD23	1:B:146:LEU:C	2.38	0.42
1:A:122:GLU:HB2	1:A:133:LEU:CD2	2.49	0.42
1:A:231:PHE:CZ	1:A:235:LEU:HD11	2.54	0.42
1:A:209:THR:HG21	1:A:308:CYS:SG	2.58	0.42
1:B:363:LEU:C	1:B:363:LEU:HD23	2.40	0.42
1:D:110:VAL:HA	1:D:132:HIS:HB2	2.00	0.42
1:D:279:GLU:H	1:D:279:GLU:CD	2.20	0.42
1:A:311:ASN:HD21	1:C:311:ASN:CB	2.23	0.42
1:C:11:SER:N	1:C:106:THR:HG23	2.33	0.42
1:A:274:ASN:HA	1:A:274:ASN:HD22	1.58	0.42
1:B:126:ARG:HG2	1:B:126:ARG:NH1	2.33	0.42
1:B:44:SER:O	1:B:48:ILE:HG13	2.19	0.42
1:D:31:ILE:HD11	1:D:81:ASN:HD21	1.83	0.42
1:C:17:ASP:HB3	1:C:24:LYS:HB2	2.01	0.42
1:A:73:LEU:HD23	1:A:73:LEU:C	2.40	0.42
1:B:31:ILE:O	1:B:31:ILE:HG23	2.18	0.42
1:D:194:VAL:HB	1:D:211:THR:CG2	2.50	0.42
1:D:284:VAL:O	1:D:284:VAL:HG13	2.18	0.42
1:C:194:VAL:HB	1:C:211:THR:CG2	2.47	0.42
1:B:23:VAL:O	1:B:86:ARG:HA	2.20	0.42
1:B:274:ASN:HA	1:B:274:ASN:HD22	1.66	0.42
1:A:207:ARG:NH1	1:C:263:LEU:HD21	2.35	0.42
1:C:363:LEU:C	1:C:363:LEU:HD23	2.40	0.41
1:C:7:VAL:HG23	3:C:1922:HOH:O	2.20	0.41
1:C:213:LEU:HD12	1:C:213:LEU:N	2.34	0.41
1:A:96:ILE:HD12	1:A:121:PHE:HZ	1.85	0.41
1:B:260:ARG:HG3	1:B:260:ARG:HH11	1.84	0.41
1:B:363:LEU:O	1:B:363:LEU:HD23	2.20	0.41
1:C:264:PRO:HG2	1:C:267:ALA:HB2	2.02	0.41
1:B:182:PRO:O	1:B:316:ARG:NH2	2.54	0.41
1:B:183:TYR:HA	1:B:184:PRO:HA	1.90	0.41
1:B:185:LEU:HD11	1:B:318:VAL:CG2	2.50	0.41
1:A:175:MET:SD	1:B:31:ILE:HG12	2.61	0.41
1:C:258:TYR:HB3	1:C:263:LEU:HB2	2.02	0.41
1:A:261:PHE:CE1	1:C:139:LEU:HD12	2.56	0.41
1:B:31:ILE:HG22	1:B:79:ARG:HB3	2.03	0.41
1:C:181:ASP:O	1:C:181:ASP:CG	2.59	0.41
1:C:92:LEU:N	1:C:93:PRO:CD	2.84	0.41
1:A:134:HIS:HB2	3:A:1679:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ASP:OD1	1:B:78:ARG:NH2	2.54	0.41
1:A:122:GLU:HB2	1:A:133:LEU:HD22	2.02	0.41
1:A:28:PHE:CZ	1:A:80:GLY:HA3	2.56	0.41
1:C:235:LEU:CD1	1:C:326:VAL:HB	2.51	0.41
1:B:233:GLU:O	1:B:237:MET:HG3	2.22	0.40
1:D:241:GLY:HA3	1:D:287:GLU:O	2.21	0.40
1:A:135:LYS:HE3	3:A:1689:HOH:O	2.21	0.40
1:B:264:PRO:HG2	1:B:267:ALA:HB2	2.04	0.40
1:D:72:ASP:OD1	1:D:79:ARG:HD2	2.22	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	347/362 (96%)	338 (97%)	9 (3%)	0	100	100
1	B	348/362 (96%)	336 (97%)	10 (3%)	2 (1%)	28	17
1	C	342/362 (94%)	329 (96%)	10 (3%)	3 (1%)	20	10
1	D	344/362 (95%)	334 (97%)	8 (2%)	2 (1%)	28	17
All	All	1381/1448 (95%)	1337 (97%)	37 (3%)	7 (0%)	32	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	109	THR
1	B	182	PRO
1	C	9	ARG
1	B	326	VAL
1	D	327	ASN
1	C	180	ASP

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Mol	Chain	Res	Type
1	D	128	ILE

5.3.2　Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/304 (98%)	295 (99%)	3 (1%)	80	79
1	B	299/304 (98%)	295 (99%)	4 (1%)	73	72
1	C	293/304 (96%)	287 (98%)	6 (2%)	60	56
1	D	293/304 (96%)	288 (98%)	5 (2%)	66	63
All	All	1183/1216 (97%)	1165 (98%)	18 (2%)	70	68

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	73	LEU
1	A	257	ASP
1	B	73	LEU
1	B	120	LYS
1	B	236	GLU
1	B	322	ASN
1	C	24	LYS
1	C	73	LEU
1	C	130	ASN
1	C	154	PHE
1	C	165	ASN
1	C	180	ASP
1	D	112	CYS
1	D	154	PHE
1	D	165	ASN
1	D	251	ARG
1	D	306	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	165	ASN
1	A	200	HIS
1	A	274	ASN
1	A	311	ASN
1	A	327	ASN
1	B	130	ASN
1	B	157	GLN
1	B	165	ASN
1	B	274	ASN
1	B	311	ASN
1	C	108	GLN
1	C	130	ASN
1	C	134	HIS
1	C	157	GLN
1	C	165	ASN
1	C	204	ASN
1	C	274	ASN
1	C	327	ASN
1	D	165	ASN
1	D	274	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1604	-	25,28,53	1.47	4 (16%)	30,40,79	1.84	4 (13%)
2	ACO	B	1704	-	25,28,53	1.52	4 (16%)	30,40,79	1.82	4 (13%)
2	ACO	C	1804	-	25,28,53	1.45	3 (12%)	30,40,79	1.76	4 (13%)
2	ACO	D	1904	-	25,28,53	1.50	5 (20%)	30,40,79	1.83	4 (13%)

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	1604	-	-	0/36/36/67	0/0/0/3
2	ACO	B	1704	-	-	0/36/36/67	0/0/0/3
2	ACO	C	1804	-	-	0/36/36/67	0/0/0/3
2	ACO	D	1904	-	-	0/36/36/67	0/0/0/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1704	ACO	C-S1P	-3.31	1.53	1.75
2	D	1904	ACO	C-S1P	-3.26	1.53	1.75
2	C	1804	ACO	C-S1P	-3.20	1.53	1.75
2	A	1604	ACO	C-S1P	-3.19	1.53	1.75
2	D	1904	ACO	C9P-N8P	2.09	1.37	1.33
2	A	1604	ACO	P1A-O3A	2.15	1.63	1.60
2	D	1904	ACO	O-C	2.25	1.32	1.21
2	A	1604	ACO	O-C	2.25	1.32	1.21
2	C	1804	ACO	O-C	2.28	1.32	1.21
2	D	1904	ACO	P1A-O3A	2.35	1.63	1.60
2	B	1704	ACO	O-C	2.47	1.33	1.21
2	B	1704	ACO	P1A-O3A	2.74	1.64	1.60
2	A	1604	ACO	CH3-C	3.32	1.65	1.50
2	D	1904	ACO	CH3-C	3.32	1.65	1.50
2	C	1804	ACO	CH3-C	3.36	1.65	1.50
2	B	1704	ACO	CH3-C	3.39	1.65	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1604	ACO	O-C-CH3	-4.81	101.62	122.88
2	C	1804	ACO	O-C-CH3	-4.81	101.63	122.88
2	D	1904	ACO	O-C-CH3	-4.75	101.89	122.88
2	B	1704	ACO	O-C-CH3	-4.65	102.33	122.88
2	C	1804	ACO	C2P-C3P-N4P	-3.06	105.75	112.49
2	B	1704	ACO	C2P-C3P-N4P	-3.04	105.79	112.49
2	D	1904	ACO	C2P-C3P-N4P	-3.01	105.86	112.49
2	A	1604	ACO	C2P-C3P-N4P	-2.93	106.04	112.49
2	A	1604	ACO	C3P-C2P-S1P	-2.71	103.37	111.23
2	C	1804	ACO	C3P-C2P-S1P	-2.53	103.88	111.23
2	B	1704	ACO	C3P-C2P-S1P	-2.45	104.11	111.23
2	D	1904	ACO	C3P-C2P-S1P	-2.40	104.25	111.23
2	C	1804	ACO	C3P-N4P-C5P	5.50	133.40	122.84
2	D	1904	ACO	C3P-N4P-C5P	5.98	134.32	122.84
2	B	1704	ACO	C3P-N4P-C5P	6.16	134.67	122.84
2	A	1604	ACO	C3P-N4P-C5P	6.33	134.99	122.84

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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	353/362 (97%)	0.32	22 (6%)	21	23	13, 27, 50, 70	0
1	B	354/362 (97%)	0.46	26 (7%)	16	17	16, 31, 53, 73	0
1	C	348/362 (96%)	0.43	24 (6%)	18	19	13, 28, 53, 68	0
1	D	348/362 (96%)	0.49	32 (9%)	10	11	16, 29, 57, 74	0
All	All	1403/1448 (96%)	0.43	104 (7%)	15	17	13, 29, 54, 74	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	128	ILE	8.4
1	A	127	THR	8.2
1	C	109	THR	8.2
1	D	126	ARG	6.4
1	B	127	THR	6.3
1	B	63	ILE	6.1
1	A	128	ILE	5.9
1	D	109	THR	5.6
1	A	63	ILE	5.5
1	B	61	THR	5.4
1	D	132	HIS	5.2
1	B	128	ILE	5.0
1	B	55	ASN	4.8
1	B	368	ASN	4.8
1	C	327	ASN	4.8
1	C	110	VAL	4.7
1	B	126	ARG	4.6
1	D	108	GLN	4.5
1	B	62	GLY	4.1
1	C	133	LEU	4.0
1	A	368	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	111	LEU	3.8
1	B	64	ARG	3.6
1	A	326	VAL	3.5
1	B	124	ASP	3.4
1	C	180	ASP	3.4
1	A	327	ASN	3.4
1	A	157	GLN	3.4
1	C	130	ASN	3.4
1	B	259	GLU	3.4
1	B	327	ASN	3.3
1	C	132	HIS	3.3
1	A	180	ASP	3.3
1	D	119	TYR	3.2
1	C	157	GLN	3.2
1	D	110	VAL	3.1
1	D	129	GLY	3.0
1	D	36	GLU	3.0
1	D	13	TRP	3.0
1	D	34	THR	3.0
1	A	297	ILE	3.0
1	A	61	THR	3.0
1	D	229	GLU	2.9
1	C	123	LYS	2.9
1	B	9	ARG	2.8
1	A	181	ASP	2.8
1	B	180	ASP	2.8
1	D	190	ILE	2.8
1	B	125	PHE	2.8
1	C	7	VAL	2.7
1	C	181	ASP	2.7
1	B	153	SER	2.7
1	D	107	LEU	2.7
1	D	55	ASN	2.7
1	C	108	GLN	2.7
1	A	126	ARG	2.7
1	B	301	ILE	2.7
1	D	282	GLU	2.7
1	B	123	LYS	2.7
1	D	213	LEU	2.7
1	C	227	GLY	2.6
1	D	278	LYS	2.6
1	D	123	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	55	ASN	2.6
1	A	259	GLU	2.6
1	A	64	ARG	2.5
1	C	278	LYS	2.5
1	B	296	THR	2.5
1	D	134	HIS	2.5
1	C	111	LEU	2.5
1	D	301	ILE	2.5
1	B	121	PHE	2.5
1	A	213	LEU	2.4
1	D	37	GLU	2.4
1	D	297	ILE	2.4
1	D	171	ARG	2.4
1	C	9	ARG	2.4
1	D	63	ILE	2.4
1	C	171	ARG	2.3
1	B	262	GLY	2.3
1	B	255	GLY	2.3
1	C	279	GLU	2.3
1	B	213	LEU	2.3
1	C	213	LEU	2.3
1	C	229	GLU	2.2
1	C	156	GLY	2.2
1	A	124	ASP	2.2
1	D	214	GLY	2.2
1	A	301	ILE	2.2
1	D	120	LYS	2.2
1	C	297	ILE	2.1
1	C	64	ARG	2.1
1	D	259	GLU	2.1
1	D	194	VAL	2.1
1	B	297	ILE	2.1
1	B	95	PHE	2.1
1	D	32	ASP	2.1
1	A	62	GLY	2.1
1	A	94	THR	2.1
1	A	90	GLN	2.1
1	A	262	GLY	2.1
1	D	105	SER	2.0
1	C	131	LEU	2.0
1	B	157	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	ACO	B	1704	29/51	0.95	0.12	-0.14	18,22,40,42	0
2	ACO	A	1604	29/51	0.96	0.12	-0.35	13,18,35,37	0
2	ACO	D	1904	29/51	0.95	0.13	-0.44	20,27,36,36	0
2	ACO	C	1804	29/51	0.96	0.12	-0.69	15,23,37,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.