



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:58 PM GMT

PDB ID : 4NB4
Title : Pantothenamide-bound Pantothenate kinase from Staphylococcus aureus
Authors : Hughes, S.J.; Antoshchenko, T.; Smil, D.; Park, H.W.
Deposited on : 2013-10-22
Resolution : 2.25 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

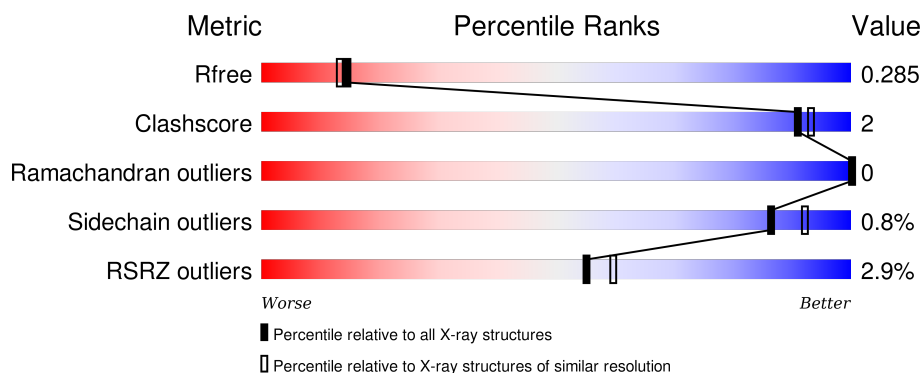
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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

Mol	Chain	Length	Quality of chain
1	A	285	<div> <div>3%</div> <div>88%</div> <div>7%</div> </div>
1	B	285	<div> <div>89%</div> <div>7%</div> </div>
1	C	285	<div> <div>%</div> <div>92%</div> <div>7%</div> </div>
1	D	285	<div> <div>4%</div> <div>87%</div> <div>6%</div> <div>7%</div> </div>
1	E	285	<div> <div>4%</div> <div>85%</div> <div>6%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	285	<div><div></div><div>7%</div><div></div><div>84%</div><div></div><div>8%</div><div>8%</div></div>
1	G	285	<div><div></div><div>%</div><div></div><div>86%</div><div></div><div>7%</div><div>7%</div></div>
1	H	285	<div><div></div><div>%</div><div></div><div>88%</div><div></div><div>6%</div><div>6%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17249 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 Type II pantothenate kinase.

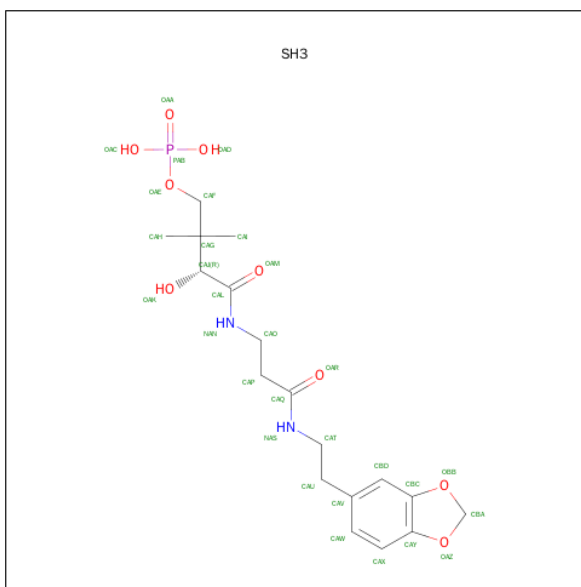
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	3	0
			2067	1308	358	395	6			
1	B	265	Total	C	N	O	S	0	3	0
			2061	1302	356	397	6			
1	C	265	Total	C	N	O	S	0	0	0
			2034	1289	350	389	6			
1	D	265	Total	C	N	O	S	0	2	0
			2053	1301	351	395	6			
1	E	259	Total	C	N	O	S	0	1	0
			1988	1258	342	382	6			
1	F	262	Total	C	N	O	S	0	1	0
			2016	1276	348	386	6			
1	G	265	Total	C	N	O	S	0	2	0
			2052	1299	354	393	6			
1	H	267	Total	C	N	O	S	0	1	0
			2053	1299	352	395	7			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	H	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 3 is N-[2-(1,3-BENZODIOXOL-5-YL)ETHYL]-N 3 -[(2R)-2-HYDROXY-3,3-DIMETHYL-4-(PHOSPHONOOXY)BUTANOYL]-BETA-ALANINAMIDE (three-letter code: SH3) (formula: $C_{18}H_{27}N_2O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 30	C 18	N 2	O 9	P 1	0	0
3	A	1	Total 30	C 18	N 2	O 9	P 1	0	0
3	C	1	Total 30	C 18	N 2	O 9	P 1	0	0
3	C	1	Total 30	C 18	N 2	O 9	P 1	0	0
3	F	1	Total 30	C 18	N 2	O 9	P 1	0	0
3	F	1	Total 30	C 18	N 2	O 9	P 1	0	0
3	G	1	Total 30	C 18	N 2	O 9	P 1	0	0
3	H	1	Total 30	C 18	N 2	O 9	P 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0

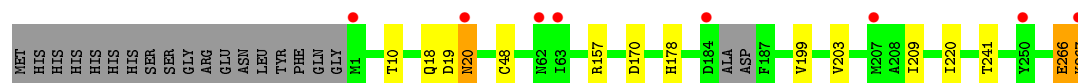
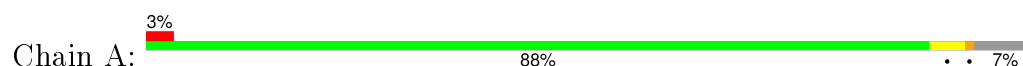
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total 58	O 58	0	0
5	B	83	Total 83	O 83	0	0
5	C	58	Total 58	O 58	0	0
5	D	42	Total 42	O 42	0	0
5	E	40	Total 40	O 40	0	0
5	F	31	Total 31	O 31	0	0
5	G	71	Total 71	O 71	0	0
5	H	78	Total 78	O 78	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: Type II pantothenate kinase



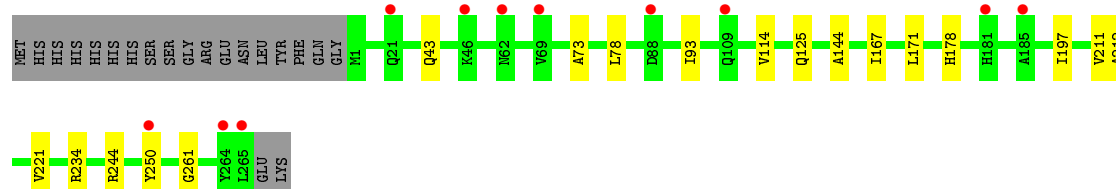
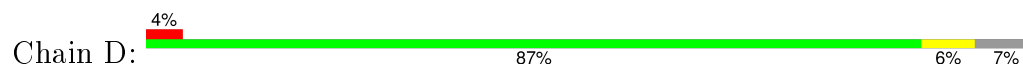
- Molecule 1: Type II pantothenate kinase



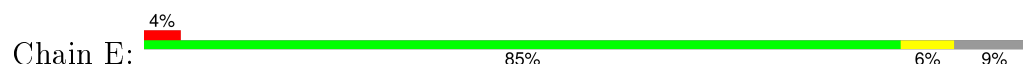
- Molecule 1: Type II pantothenate kinase



- Molecule 1: Type II pantothenate kinase

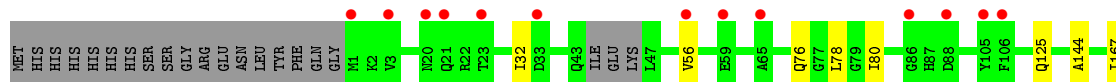
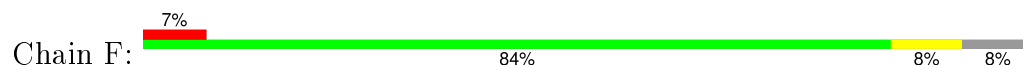


- Molecule 1: Type II pantothenate kinase

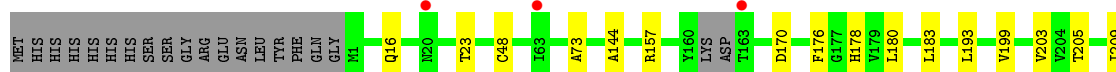
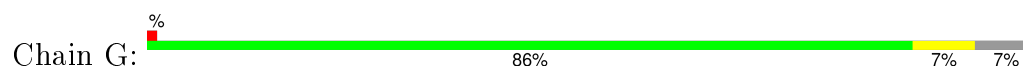




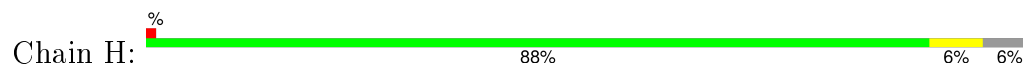
- Molecule 1: Type II pantothenate kinase



- Molecule 1: Type II pantothenate kinase



- Molecule 1: Type II pantothenate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.01Å 70.74Å 143.12Å 90.00° 90.64° 90.00°	Depositor
Resolution (Å)	39.91 – 2.25 39.88 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.91-2.25) 96.3 (39.88-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.230 , 0.284 0.233 , 0.285	Depositor DCC
R_{free} test set	4896 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 5.1	EDS
Estimated twinning fraction	0.185 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 97508 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17249	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SH3, ADP

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	1/2102 (0.0%)	0.51	1/2844 (0.0%)
1	B	0.31	0/2096	0.50	0/2839
1	C	0.32	0/2067	0.49	0/2795
1	D	0.33	0/2089	0.49	0/2832
1	E	0.31	0/2020	0.48	0/2733
1	F	0.30	0/2051	0.48	0/2779
1	G	0.33	0/2087	0.51	0/2826
1	H	0.32	0/2088	0.51	0/2828
All	All	0.32	1/16600 (0.0%)	0.50	1/22476 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	GLU	CD-OE1	-5.27	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ASN	CB-CA-C	-6.19	98.02	110.40

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	2067	0	2053	9	0
1	B	2061	0	2034	6	0
1	C	2034	0	2025	2	0
1	D	2053	0	2035	11	0
1	E	1988	0	1973	13	0
1	F	2016	0	1996	16	0
1	G	2052	0	2035	11	0
1	H	2053	0	2038	14	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
3	A	60	0	52	0	0
3	C	60	0	52	0	0
3	F	60	0	53	0	0
3	G	30	0	26	0	0
3	H	30	0	26	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	58	0	0	0	0
5	B	83	0	0	0	0
5	C	58	0	0	0	0
5	D	42	0	0	0	0
5	E	40	0	0	0	0
5	F	31	0	0	0	0
5	G	71	0	0	0	0
5	H	78	0	0	2	0
All	All	17249	0	16494	73	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 2.

All (73) 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:H:46:LYS:HG2	1:H:266:GLU:OE2	1.47	1.13
1:E:46:LYS:HE3	1:E:266:GLU:OE2	1.62	0.99
1:H:46:LYS:HG2	1:H:266:GLU:CD	1.83	0.97
1:E:46:LYS:CE	1:E:266:GLU:OE2	2.36	0.73
1:D:93:ILE:HD13	1:D:211:VAL:HG13	1.75	0.69
1:A:48:CYS:SG	1:A:266:GLU:HG3	2.35	0.67
1:G:205:THR:HG22	1:G:209:ILE:HD13	1.81	0.62
1:A:209:ILE:HD11	1:A:241:THR:HA	1.83	0.60
1:H:48:CYS:SG	1:H:266:GLU:HB2	2.42	0.59
1:G:157:ARG:NH2	1:G:170:ASP:OD1	2.37	0.58
1:E:117:ILE:HD11	1:F:203:VAL:HG22	1.88	0.56
1:D:114:VAL:CG2	1:D:211:VAL:HG21	2.35	0.55
1:H:46:LYS:CG	1:H:266:GLU:OE2	2.39	0.55
1:E:113:ARG:HD3	1:F:167:ILE:HD11	1.89	0.54
1:F:80:ILE:HD11	1:F:264:TYR:CD2	2.42	0.54
1:E:114:VAL:CG2	1:E:211:VAL:HG21	2.38	0.53
1:F:78:LEU:HD13	1:F:223:ILE:HG21	1.93	0.51
1:E:125:GLN:HB3	1:F:180:LEU:HD11	1.93	0.50
1:H:151:THR:HG23	1:H:152:ILE:HG13	1.94	0.50
1:E:126:GLY:HA3	1:F:176:PHE:O	2.12	0.49
1:D:93:ILE:HD12	1:D:212:ALA:HA	1.93	0.49
1:F:199:VAL:O	1:F:203:VAL:HG23	2.12	0.49
1:G:180:LEU:HD23	1:G:183:LEU:HD21	1.94	0.49
1:H:38:TRP:O	1:H:42:GLN:HG2	2.14	0.48
1:E:114:VAL:HG21	1:E:211:VAL:HG21	1.96	0.48
1:D:167:ILE:HG22	1:D:171:LEU:HD12	1.97	0.47
1:H:70:GLU:HG2	5:H:439:HOH:O	2.15	0.47
1:E:113:ARG:CD	1:F:167:ILE:HD11	2.44	0.47
1:G:199:VAL:O	1:G:203:VAL:HG23	2.14	0.47
1:C:180:LEU:HD11	1:D:125:GLN:HB3	1.97	0.47
1:G:73:ALA:O	1:G:261:GLY:HA3	2.15	0.47
1:A:209:ILE:HD13	1:A:220:ILE:CD1	2.44	0.46
1:G:16:GLN:HB2	1:G:23:THR:HB	1.97	0.46
1:H:46:LYS:HE2	1:H:266:GLU:OE1	2.16	0.46
1:B:209:ILE:HD13	1:B:244:ARG:HG3	1.98	0.46
1:H:151:THR:HG21	5:H:435:HOH:O	2.15	0.46
1:G:176:PHE:O	1:H:126:GLY:HA3	2.16	0.46
1:G:237:VAL:CG2	1:G:250:TYR:OH	2.64	0.46
1:D:78:LEU:HD11	1:D:221:VAL:HG11	1.98	0.46
1:G:209:ILE:HD11	1:G:241:THR:HA	1.99	0.45
1:E:180:LEU:HD11	1:F:125:GLN:HB3	1.98	0.45
1:A:18:GLN:O	1:A:19:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ARG:NH1	1:D:250[B]:TYR:CE1	2.85	0.44
1:F:265:LEU:C	1:F:265:LEU:HD12	2.38	0.44
1:A:19:ASP:O	1:A:20:ASN:HB2	2.18	0.44
1:A:266:GLU:O	1:A:267:LYS:HG2	2.18	0.43
1:B:11:LEU:HD22	1:B:26:THR:CG2	2.47	0.43
1:F:225:SER:HA	1:F:228[B]:HIS:CE1	2.53	0.43
1:F:32:ILE:HD13	1:F:56:VAL:HG11	2.01	0.43
1:D:167:ILE:CG2	1:D:171:LEU:HD12	2.49	0.43
1:D:73:ALA:O	1:D:261:GLY:HA3	2.19	0.43
1:G:48:CYS:SG	1:G:266:GLU:HB2	2.59	0.43
1:D:144:ALA:HB1	1:D:197:ILE:HD12	2.01	0.43
1:D:114:VAL:HG21	1:D:211:VAL:HG21	1.99	0.42
1:F:234:ARG:HD3	1:F:250:TYR:CE2	2.53	0.42
1:E:188:THR:CG2	1:E:191:ASN:CG	2.88	0.42
1:C:103:LEU:HD11	1:C:207:MET:HB3	2.01	0.42
1:F:78:LEU:HD11	1:F:221:VAL:HG11	2.02	0.42
1:E:237:VAL:HG23	1:E:250:TYR:OH	2.20	0.42
1:B:33:ASP:O	1:B:37:GLU:HG2	2.20	0.41
1:F:144:ALA:HB1	1:F:197:ILE:HD12	2.02	0.41
1:E:57:ILE:O	1:E:61:ILE:HB	2.20	0.41
1:H:102:SER:HB2	3:H:302:SH3:OAM	2.20	0.41
1:A:157[A]:ARG:NH2	1:A:170:ASP:OD1	2.53	0.41
1:A:10:THR:HG21	2:A:301:ADP:H3'	2.02	0.41
1:G:144:ALA:HB2	1:G:193:LEU:HB3	2.03	0.41
1:H:144:ALA:HB1	1:H:197:ILE:HD12	2.03	0.41
1:B:265:LEU:HA	1:B:265:LEU:HD23	1.87	0.41
1:B:78:LEU:HD11	1:B:221:VAL:HG11	2.03	0.40
1:A:199:VAL:O	1:A:203:VAL:HG23	2.21	0.40
1:F:76:GLN:HG2	1:F:264:TYR:CD1	2.56	0.40
1:H:78:LEU:HD11	1:H:221:VAL:HG11	2.04	0.40
1:B:133:GLN:HB3	1:H:247:LYS:HE2	2.02	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	264/285 (93%)	257 (97%)	7 (3%)	0	100	100
1	B	264/285 (93%)	258 (98%)	6 (2%)	0	100	100
1	C	259/285 (91%)	254 (98%)	5 (2%)	0	100	100
1	D	265/285 (93%)	259 (98%)	6 (2%)	0	100	100
1	E	254/285 (89%)	248 (98%)	6 (2%)	0	100	100
1	F	259/285 (91%)	247 (95%)	12 (5%)	0	100	100
1	G	263/285 (92%)	256 (97%)	7 (3%)	0	100	100
1	H	266/285 (93%)	262 (98%)	4 (2%)	0	100	100
All	All	2094/2280 (92%)	2041 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	219/233 (94%)	217 (99%)	2 (1%)	84	91
1	B	218/233 (94%)	217 (100%)	1 (0%)	92	95
1	C	215/233 (92%)	214 (100%)	1 (0%)	92	95
1	D	217/233 (93%)	214 (99%)	3 (1%)	74	84
1	E	210/233 (90%)	207 (99%)	3 (1%)	74	84
1	F	213/233 (91%)	212 (100%)	1 (0%)	92	95
1	G	217/233 (93%)	216 (100%)	1 (0%)	92	95
1	H	217/233 (93%)	215 (99%)	2 (1%)	84	91
All	All	1726/1864 (93%)	1712 (99%)	14 (1%)	86	92

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
1	A	267	LYS
1	B	178	HIS
1	C	178	HIS
1	D	43	GLN
1	D	178	HIS
1	D	244	ARG
1	E	112	ARG
1	E	157	ARG
1	E	178	HIS
1	F	178	HIS
1	G	178	HIS
1	H	88	ASP
1	H	178	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	C	158	HIS
1	D	43	GLN
1	D	76	GLN
1	D	139	GLN
1	E	125	GLN
1	F	42	GLN
1	F	109	GLN
1	F	150	ASN
1	G	76	GLN
1	G	158	HIS
1	H	158	HIS

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 ⓘ

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ADP	A	301	4	22,29,29	1.06	1 (4%)	27,45,45	1.87	3 (11%)
3	SH3	A	302	4	28,31,31	1.35	4 (14%)	39,44,44	1.06	4 (10%)
3	SH3	A	303	4	28,31,31	1.42	7 (25%)	39,44,44	1.39	6 (15%)
2	ADP	B	301	4	22,29,29	1.05	1 (4%)	27,45,45	1.83	1 (3%)
2	ADP	C	301	4	22,29,29	1.06	1 (4%)	27,45,45	1.92	6 (22%)
3	SH3	C	302	4	28,31,31	1.30	6 (21%)	39,44,44	1.33	5 (12%)
3	SH3	C	303	4	28,31,31	1.36	4 (14%)	39,44,44	1.16	4 (10%)
2	ADP	D	301	4	22,29,29	1.15	2 (9%)	27,45,45	1.99	3 (11%)
2	ADP	E	301	4	22,29,29	1.11	3 (13%)	27,45,45	1.84	2 (7%)
2	ADP	F	301	4	22,29,29	1.09	2 (9%)	27,45,45	1.81	4 (14%)
3	SH3	F	302	4	28,31,31	1.33	6 (21%)	39,44,44	1.14	5 (12%)
3	SH3	F	303	4	28,31,31	1.35	5 (17%)	39,44,44	1.20	5 (12%)
2	ADP	G	301	4	22,29,29	1.08	2 (9%)	27,45,45	1.87	4 (14%)
3	SH3	G	302	4	28,31,31	1.28	6 (21%)	39,44,44	1.28	5 (12%)
2	ADP	H	301	4	22,29,29	1.12	2 (9%)	27,45,45	1.93	4 (14%)
3	SH3	H	302	4	28,31,31	1.34	5 (17%)	39,44,44	1.69	6 (15%)

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	ADP	A	301	4	-	0/12/32/32	0/3/3/3
3	SH3	A	302	4	-	0/29/35/35	0/2/2/2
3	SH3	A	303	4	-	0/29/35/35	0/2/2/2
2	ADP	B	301	4	-	0/12/32/32	0/3/3/3
2	ADP	C	301	4	-	0/12/32/32	0/3/3/3
3	SH3	C	302	4	-	0/29/35/35	0/2/2/2
3	SH3	C	303	4	-	0/29/35/35	0/2/2/2
2	ADP	D	301	4	-	0/12/32/32	0/3/3/3
2	ADP	E	301	4	-	0/12/32/32	0/3/3/3
2	ADP	F	301	4	-	0/12/32/32	0/3/3/3
3	SH3	F	302	4	-	0/29/35/35	0/2/2/2
3	SH3	F	303	4	-	0/29/35/35	0/2/2/2
2	ADP	G	301	4	-	0/12/32/32	0/3/3/3
3	SH3	G	302	4	-	0/29/35/35	0/2/2/2
2	ADP	H	301	4	-	0/12/32/32	0/3/3/3
3	SH3	H	302	4	-	1/29/35/35	0/2/2/2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	302	SH3	CAU-CAV	-3.62	1.41	1.51
3	A	303	SH3	CAU-CAV	-3.60	1.41	1.51
3	F	303	SH3	CAU-CAV	-3.52	1.41	1.51
3	A	302	SH3	CAU-CAV	-3.50	1.41	1.51
3	C	303	SH3	CAU-CAV	-3.44	1.41	1.51
3	C	302	SH3	CAU-CAV	-3.37	1.42	1.51
3	H	302	SH3	CAU-CAV	-3.27	1.42	1.51
3	G	302	SH3	CAU-CAV	-3.24	1.42	1.51
3	A	302	SH3	CAX-CAY	-2.75	1.33	1.39
3	G	302	SH3	CAX-CAY	-2.74	1.33	1.39
3	F	303	SH3	CAX-CAY	-2.65	1.34	1.39
3	C	303	SH3	CAX-CAY	-2.63	1.34	1.39
3	C	302	SH3	CAX-CAY	-2.60	1.34	1.39
3	F	302	SH3	CAX-CAY	-2.58	1.34	1.39
3	H	302	SH3	CAX-CAY	-2.50	1.34	1.39
3	C	303	SH3	CBD-CBC	-2.50	1.34	1.38
3	A	303	SH3	CBD-CBC	-2.48	1.34	1.38
3	A	302	SH3	CBD-CBC	-2.42	1.34	1.38
3	A	303	SH3	CAX-CAY	-2.38	1.34	1.39
3	G	302	SH3	CBD-CBC	-2.34	1.34	1.38
3	A	303	SH3	CAY-CBC	-2.31	1.32	1.39
3	F	303	SH3	CAY-CBC	-2.15	1.33	1.39
3	C	303	SH3	CAY-CBC	-2.14	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	303	SH3	CBD-CBC	-2.14	1.34	1.38
3	C	302	SH3	CAY-CBC	-2.13	1.33	1.39
3	H	302	SH3	CBD-CBC	-2.12	1.34	1.38
3	H	302	SH3	CAY-CBC	-2.11	1.33	1.39
3	F	302	SH3	CAY-CBC	-2.07	1.33	1.39
3	C	302	SH3	CBD-CBC	-2.06	1.34	1.38
3	G	302	SH3	CAY-CBC	-2.04	1.33	1.39
3	F	302	SH3	CBD-CBC	-2.04	1.34	1.38
2	E	301	ADP	O4'-C1'	2.01	1.43	1.41
3	F	302	SH3	PAB-OAD	2.01	1.61	1.54
3	G	302	SH3	PAB-OAC	2.03	1.62	1.54
3	C	302	SH3	PAB-OAD	2.10	1.62	1.54
2	E	301	ADP	C2-N3	2.16	1.36	1.32
3	F	303	SH3	OAZ-CBA	2.20	1.47	1.43
3	G	302	SH3	OAZ-CBA	2.21	1.47	1.43
3	A	303	SH3	PAB-OAC	2.21	1.62	1.54
2	F	301	ADP	O4'-C1'	2.22	1.44	1.41
3	H	302	SH3	CAP-CAQ	2.25	1.55	1.51
3	F	302	SH3	PAB-OAC	2.26	1.62	1.54
3	C	302	SH3	PAB-OAC	2.29	1.62	1.54
3	A	303	SH3	PAB-OAD	2.31	1.63	1.54
3	A	303	SH3	OAZ-CBA	2.33	1.47	1.43
2	G	301	ADP	O4'-C1'	2.33	1.44	1.41
2	H	301	ADP	O4'-C1'	2.41	1.44	1.41
2	D	301	ADP	O4'-C1'	2.65	1.44	1.41
3	A	302	SH3	OAZ-CBA	2.70	1.48	1.43
2	B	301	ADP	C5-C4	2.97	1.47	1.40
2	G	301	ADP	C5-C4	3.06	1.47	1.40
2	A	301	ADP	C5-C4	3.07	1.47	1.40
2	F	301	ADP	C5-C4	3.14	1.47	1.40
2	E	301	ADP	C5-C4	3.15	1.47	1.40
2	C	301	ADP	C5-C4	3.16	1.47	1.40
2	H	301	ADP	C5-C4	3.23	1.47	1.40
2	D	301	ADP	C5-C4	3.24	1.47	1.40

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	ADP	N3-C2-N1	-8.28	122.55	128.89
2	H	301	ADP	N3-C2-N1	-8.05	122.73	128.89
2	A	301	ADP	N3-C2-N1	-7.85	122.89	128.89
2	E	301	ADP	N3-C2-N1	-7.81	122.92	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ADP	N3-C2-N1	-7.64	123.05	128.89
2	C	301	ADP	N3-C2-N1	-7.53	123.12	128.89
2	G	301	ADP	N3-C2-N1	-7.47	123.17	128.89
2	F	301	ADP	N3-C2-N1	-7.14	123.43	128.89
3	A	303	SH3	OAZ-CBA-OB	-4.51	100.49	108.12
3	C	303	SH3	OAZ-CBA-OB	-4.37	100.73	108.12
3	C	302	SH3	OAZ-CBA-OB	-4.35	100.76	108.12
3	H	302	SH3	OAZ-CBA-OB	-3.67	101.92	108.12
3	F	303	SH3	OAZ-CBA-OB	-3.62	101.99	108.12
3	F	302	SH3	OAZ-CBA-OB	-3.48	102.23	108.12
3	G	302	SH3	OAZ-CBA-OB	-3.29	102.56	108.12
3	H	302	SH3	OAM-CAL-NAN	-3.24	116.59	123.08
3	F	302	SH3	CAU-CAT-NAS	-3.18	104.22	111.97
3	F	303	SH3	CAU-CAT-NAS	-3.15	104.28	111.97
3	G	302	SH3	CAU-CAT-NAS	-3.06	104.51	111.97
3	H	302	SH3	CAP-CAO-NAN	-3.06	105.18	111.88
2	D	301	ADP	C4-C5-N7	-3.04	106.68	109.48
3	G	302	SH3	CAO-CAP-CAQ	-3.02	107.33	112.31
2	F	301	ADP	C4-C5-N7	-2.87	106.84	109.48
3	G	302	SH3	CAT-CAU-CAV	-2.81	107.01	112.83
2	A	301	ADP	C4-C5-N7	-2.76	106.94	109.48
3	C	302	SH3	CAO-CAP-CAQ	-2.75	107.78	112.31
3	A	302	SH3	CAT-CAU-CAV	-2.75	107.14	112.83
2	H	301	ADP	C4-C5-N7	-2.74	106.96	109.48
3	C	302	SH3	CAU-CAT-NAS	-2.59	105.64	111.97
2	H	301	ADP	O3A-PA-O5'	-2.59	96.06	102.94
3	A	302	SH3	OAZ-CBA-OB	-2.57	103.78	108.12
3	A	303	SH3	CAT-CAU-CAV	-2.53	107.57	112.83
2	C	301	ADP	PA-O3A-PB	-2.53	124.20	132.67
3	A	303	SH3	CAU-CAT-NAS	-2.52	105.83	111.97
3	C	302	SH3	CAT-CAU-CAV	-2.51	107.62	112.83
3	A	302	SH3	CAU-CAT-NAS	-2.50	105.89	111.97
2	C	301	ADP	C4-C5-N7	-2.46	107.22	109.48
3	A	303	SH3	CAO-CAP-CAQ	-2.39	108.37	112.31
2	G	301	ADP	C4-C5-N7	-2.36	107.31	109.48
2	C	301	ADP	O3A-PA-O5'	-2.27	96.91	102.94
3	F	302	SH3	CAO-CAP-CAQ	-2.25	108.60	112.31
3	F	302	SH3	CAT-CAU-CAV	-2.20	108.28	112.83
2	F	301	ADP	PA-O3A-PB	-2.16	125.41	132.67
3	F	303	SH3	CAT-CAU-CAV	-2.06	108.57	112.83
3	F	303	SH3	CAO-CAP-CAQ	-2.05	108.93	112.31
2	E	301	ADP	C4-C5-N7	-2.04	107.60	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	SH3	CAU-CAT-NAS	-2.04	107.00	111.97
3	C	303	SH3	CAT-CAU-CAV	-2.04	108.61	112.83
2	G	301	ADP	C1'-N9-C4	2.02	129.99	126.94
2	D	301	ADP	O4'-C1'-N9	2.04	112.36	108.10
2	C	301	ADP	C1'-N9-C4	2.05	130.03	126.94
2	C	301	ADP	C2'-C1'-N9	2.09	117.48	114.29
2	H	301	ADP	O3B-PB-O2B	2.16	115.59	107.38
2	F	301	ADP	O3B-PB-O2B	2.20	115.77	107.38
2	A	301	ADP	C1'-N9-C4	2.25	130.33	126.94
3	A	303	SH3	OAZ-CAY-CAX	2.25	131.55	127.96
3	H	302	SH3	CAO-CAP-CAQ	2.28	116.07	112.31
3	G	302	SH3	OAE-PAB-OAA	2.33	113.08	107.14
2	G	301	ADP	O3B-PB-O2B	2.34	116.31	107.38
3	F	302	SH3	OAE-PAB-OAA	2.36	113.14	107.14
3	F	303	SH3	OAE-PAB-OAA	2.41	113.27	107.14
3	A	302	SH3	OAE-PAB-OAA	2.43	113.33	107.14
3	C	303	SH3	OAE-PAB-OAA	2.54	113.61	107.14
3	A	303	SH3	OAE-PAB-OAA	2.96	114.68	107.14
3	C	302	SH3	OAE-PAB-OAA	3.09	115.01	107.14
3	H	302	SH3	CAJ-CAL-NAN	4.19	125.75	116.47
3	H	302	SH3	CAO-NAN-CAL	5.70	133.81	122.53

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	302	SH3	CAJ-CAL-NAN-CAO

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ADP	1	0
3	H	302	SH3	1	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, 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	265/285 (92%)	0.11	8 (3%) 54 58	8, 18, 33, 53	1 (0%)
1	B	265/285 (92%)	-0.04	1 (0%) 93 93	8, 15, 30, 38	0
1	C	265/285 (92%)	0.14	4 (1%) 76 79	11, 20, 34, 53	0
1	D	265/285 (92%)	0.37	11 (4%) 40 44	12, 26, 48, 65	0
1	E	259/285 (90%)	0.26	11 (4%) 40 44	15, 26, 41, 48	0
1	F	262/285 (91%)	0.55	19 (7%) 18 19	16, 31, 53, 56	0
1	G	265/285 (92%)	-0.01	3 (1%) 82 84	7, 16, 30, 44	0
1	H	267/285 (93%)	0.03	4 (1%) 76 79	9, 16, 34, 43	0
All	All	2113/2280 (92%)	0.18	61 (2%) 55 60	7, 20, 41, 65	1 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	264	TYR	6.2
1	F	186	ASP	5.0
1	D	250[A]	TYR	4.7
1	E	157	ARG	4.7
1	C	267	LYS	4.5
1	C	20	ASN	4.3
1	D	21	GLN	4.0
1	D	265	LEU	3.9
1	F	21	GLN	3.9
1	A	250	TYR	3.9
1	A	20	ASN	3.6
1	C	266	GLU	3.6
1	C	264	TYR	3.5
1	F	185	ALA	3.5
1	E	186	ASP	3.4
1	F	86	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	207	MET	3.3
1	F	33	ASP	3.3
1	E	266	GLU	3.2
1	G	163	THR	3.2
1	F	65	ALA	3.0
1	D	185	ALA	3.0
1	D	62	ASN	2.9
1	G	20	ASN	2.9
1	A	63	ILE	2.8
1	H	30	LYS	2.7
1	F	20	ASN	2.7
1	F	183	LEU	2.7
1	F	23	THR	2.6
1	E	19	ASP	2.5
1	F	250	TYR	2.5
1	E	170	ASP	2.5
1	F	88	ASP	2.5
1	D	88	ASP	2.5
1	D	69	VAL	2.5
1	A	184	ASP	2.5
1	F	1	MET	2.4
1	H	20	ASN	2.4
1	H	61	ILE	2.4
1	D	109	GLN	2.4
1	E	156	VAL	2.3
1	E	166	PRO	2.3
1	F	106	PHE	2.3
1	F	182	HIS	2.3
1	F	3	VAL	2.3
1	F	56	VAL	2.3
1	A	62	ASN	2.3
1	E	90	ALA	2.2
1	H	62	ASN	2.2
1	E	43	GLN	2.2
1	D	46	LYS	2.2
1	D	181	HIS	2.2
1	B	162	ASP	2.2
1	F	59	GLU	2.2
1	E	140	LEU	2.1
1	A	1	MET	2.1
1	G	63	ILE	2.1
1	E	146	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	105	TYR	2.0
1	A	267	LYS	2.0
1	F	264	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	C	304	1/1	0.90	0.11	1.35	13,13,13,13	0
3	SH3	A	302	30/30	0.94	0.13	0.40	12,13,14,14	0
2	ADP	F	301	27/27	0.93	0.14	0.10	22,25,33,34	0
2	ADP	C	301	27/27	0.96	0.11	-0.14	10,10,11,11	0
3	SH3	C	303	30/30	0.93	0.13	-0.16	16,19,21,21	0
3	SH3	F	303	30/30	0.93	0.13	-0.27	20,23,31,32	0
2	ADP	H	301	27/27	0.96	0.11	-0.28	12,12,13,13	0
3	SH3	H	302	30/30	0.94	0.12	-0.32	12,12,13,13	0
3	SH3	G	302	30/30	0.95	0.11	-0.42	7,8,10,10	0
3	SH3	A	303	30/30	0.94	0.11	-0.53	12,13,14,14	0
2	ADP	A	301	27/27	0.95	0.11	-0.55	12,12,13,13	0
3	SH3	C	302	30/30	0.94	0.11	-0.57	13,15,17,17	0
2	ADP	G	301	27/27	0.97	0.10	-0.58	7,8,9,9	0
2	ADP	D	301	27/27	0.95	0.11	-0.64	15,16,17,18	0
2	ADP	E	301	27/27	0.95	0.11	-0.73	16,17,18,18	0
4	MG	G	303	1/1	0.97	0.11	-0.95	2,2,2,2	0
3	SH3	F	302	30/30	0.94	0.10	-1.48	14,16,16,16	0
2	ADP	B	301	27/27	0.97	0.09	-1.80	9,9,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	E	302	1/1	0.88	0.07	-2.08	25,25,25,25	0
4	MG	A	304	1/1	0.97	0.05	-2.95	8,8,8,8	0
4	MG	F	304	1/1	0.85	0.16	-	22,22,22,22	0
4	MG	D	302	1/1	0.82	0.08	-	19,19,19,19	0
4	MG	H	303	1/1	0.98	0.07	-	9,9,9,9	0
4	MG	B	302	1/1	0.96	0.09	-	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.