



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:42 PM GMT

PDB ID : 3RT0
Title : Crystal structure of PYL10-HAB1 complex in the absence of abscisic acid (ABA)
Authors : Hao, Q.; Yin, P.; Li, W.; Wang, L.; Yan, C.; Wang, J.; Yan, N.
Deposited on : 2011-05-02
Resolution : 2.11 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

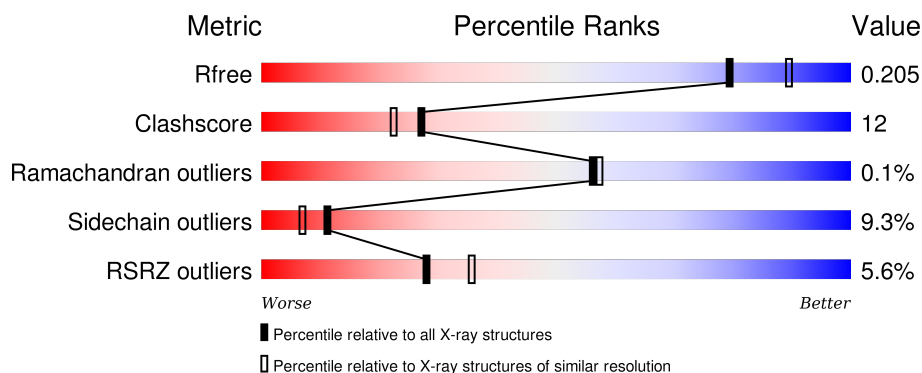
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

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	340	<div> <div>3%</div> <div>75%</div> <div>17%</div> <div>• •</div> </div>
1	B	340	<div> <div>5%</div> <div>75%</div> <div>15%</div> <div>• 8%</div> </div>
2	C	183	<div> <div>10%</div> <div>67%</div> <div>21%</div> <div>5% • 6%</div> </div>
2	D	183	<div> <div>5%</div> <div>67%</div> <div>15%</div> <div>• 14%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	B	512	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8239 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 Protein phosphatase 2C 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	7	0
			2612	1638	467	488	19			
1	B	314	Total	C	N	O	S	0	9	0
			2506	1576	444	468	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	SER	CYS	ENGINEERED MUTATION	UNP Q9CAJ0
B	274	SER	CYS	ENGINEERED MUTATION	UNP Q9CAJ0

- Molecule 2 is a protein called Absciscic acid receptor PYL10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	172	Total	C	N	O	S	0	1	0
			1369	859	237	269	4			
2	D	158	Total	C	N	O	S	0	0	0
			1243	782	217	240	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	162	SER	CYS	ENGINEERED MUTATION	UNP Q8H1R0
D	162	SER	CYS	ENGINEERED MUTATION	UNP Q8H1R0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

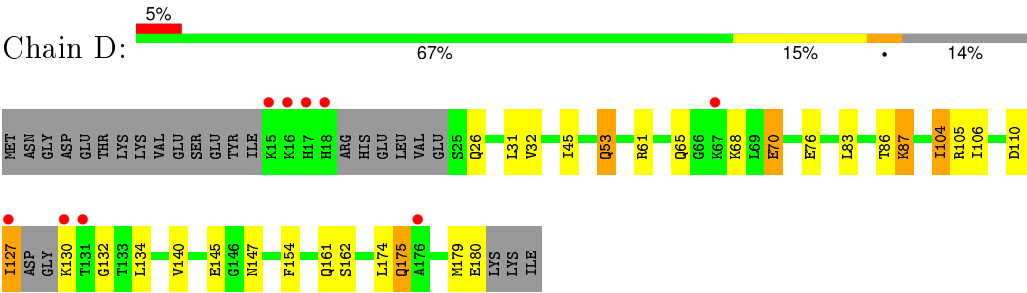
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	221	Total 221	O 221	0	0
4	B	170	Total 170	O 170	0	0
4	C	58	Total 58	O 58	0	0
4	D	58	Total 58	O 58	0	0

- Molecule 1: Protein phosphatase 2C 16





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.77Å 83.50Å 88.54Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	32.50 – 2.11 32.50 – 2.11	Depositor EDS
% Data completeness (in resolution range)	95.2 (32.50-2.11) 98.7 (32.50-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.3_473)	Depositor
R, R_{free}	0.173 , 0.207 0.175 , 0.205	Depositor DCC
R_{free} test set	2934 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 57980 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8239	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.08 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.0061e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.40	0/2660	0.56	0/3585
1	B	0.39	0/2551	0.55	1/3441 (0.0%)
2	C	0.34	0/1391	0.46	0/1878
2	D	0.35	0/1261	0.48	0/1699
All	All	0.38	0/7863	0.53	1/10603 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	429	LEU	CA-CB-CG	5.39	127.70	115.30

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	2612	0	2600	62	0
1	B	2506	0	2495	47	0
2	C	1369	0	1374	56	1
2	D	1243	0	1262	24	1
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	221	0	0	11	0
4	B	170	0	0	3	0
4	C	58	0	0	4	0
4	D	58	0	0	0	0
All	All	8239	0	7731	186	1

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 12.

All (186) 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)
2:C:16:LYS:HE3	2:C:17:HIS:NE2	1.48	1.24
2:C:19:ARG:HH11	2:C:19:ARG:HG2	1.10	1.17
2:D:126:THR:C	2:D:127:ILE:HG13	1.65	1.11
1:A:449:ARG:HG2	1:A:453:MET:HE3	1.33	1.10
1:A:509:THR:O	1:A:510:ARG:HB2	1.54	1.05
1:A:376:GLU:OE1	4:A:730:HOH:O	1.77	1.03
2:D:53:GLN:NE2	2:D:53:GLN:H	1.59	1.00
1:A:449:ARG:HG2	1:A:453:MET:CE	1.92	0.99
2:D:53:GLN:HE21	2:D:53:GLN:N	1.59	0.98
1:B:376:GLU:OE1	4:B:682:HOH:O	1.84	0.96
2:D:126:THR:O	2:D:127:ILE:HG13	1.65	0.96
1:B:265:GLU:OE2	1:B:268:ARG:NH1	1.99	0.95
2:C:53:GLN:HE21	2:C:53:GLN:H	0.99	0.95
2:D:126:THR:HA	2:D:130:LYS:O	1.66	0.95
1:A:487:GLN:OE1	4:A:733:HOH:O	1.85	0.95
1:B:301[A]:ILE:HA	1:B:320:VAL:HG13	1.48	0.92
2:C:16:LYS:HE3	2:C:17:HIS:HE2	1.22	0.92
2:C:16:LYS:CE	2:C:17:HIS:NE2	2.36	0.87
1:A:278:THR:HG23	4:A:632:HOH:O	1.76	0.86
2:D:106:ILE:HG21	2:D:111:HIS:CE1	2.11	0.84
2:D:126:THR:O	2:D:127:ILE:CG1	2.25	0.84
1:B:301[B]:ILE:HA	1:B:320:VAL:HG13	1.61	0.83
2:C:53:GLN:NE2	2:C:53:GLN:H	1.75	0.83
1:A:217:ILE:HG22	1:A:221:MET:HG3	1.59	0.82
2:C:32:VAL:HG13	2:C:134:LEU:HD11	1.60	0.81
2:C:19:ARG:HG2	2:C:19:ARG:NH1	1.89	0.80
2:D:32:VAL:HG13	2:D:134:LEU:HD11	1.62	0.79
2:C:53:GLN:HE21	2:C:53:GLN:N	1.79	0.78
2:C:173:ARG:NH1	4:C:213:HOH:O	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:THR:HG23	1:B:233:HIS:ND1	2.00	0.77
1:A:301:ILE:HA	1:A:320:VAL:HG13	1.66	0.77
1:A:418:MET:HE1	4:A:722:HOH:O	1.85	0.76
1:B:394:LEU:HG	1:B:396[B]:MET:SD	2.25	0.75
1:A:466:ARG:HD2	4:A:524:HOH:O	1.87	0.73
2:C:19:ARG:HH11	2:C:19:ARG:CG	1.93	0.73
2:D:126:THR:CA	2:D:130:LYS:O	2.36	0.72
2:D:175:GLN:HA	2:D:175:GLN:HE21	1.55	0.72
1:B:265:GLU:CD	1:B:268:ARG:HH12	1.93	0.71
1:B:403:ARG:HA	1:B:406:LYS:HD2	1.71	0.71
2:C:16:LYS:HE3	2:C:17:HIS:CD2	2.25	0.71
2:C:24:GLU:OE1	2:C:24:GLU:HA	1.90	0.71
2:C:26:GLN:CG	2:C:142:ASP:OD1	2.40	0.70
1:A:291:THR:O	1:A:295:LEU:HD23	1.89	0.70
1:A:214:LYS:HD2	1:A:233:HIS:CE1	2.27	0.69
1:B:297:VAL:O	1:B:301[A]:ILE:HG23	1.93	0.69
1:B:271:ASP:O	1:B:271:ASP:CG	2.30	0.68
2:C:26:GLN:HG2	2:C:142:ASP:OD1	1.94	0.68
2:C:16:LYS:CE	2:C:17:HIS:CD2	2.76	0.67
1:A:192[A]:THR:H	1:A:475:GLN:HE22	1.41	0.67
1:A:192[B]:THR:H	1:A:475:GLN:HE22	1.43	0.67
2:C:32:VAL:HG22	2:C:136:ILE:HG12	1.76	0.66
1:B:285:GLN:O	1:B:289[A]:VAL:HG12	1.96	0.65
1:B:250:VAL:HG23	1:B:325:VAL:HG22	1.78	0.65
1:B:181:VAL:HA	1:B:184:LEU:HD12	1.79	0.65
2:C:49:PHE:HD1	2:C:104:ILE:HD11	1.61	0.64
1:A:403:ARG:HA	1:A:406:LYS:HD2	1.80	0.64
2:D:32:VAL:CG1	2:D:134:LEU:HD11	2.26	0.64
2:C:9:VAL:O	2:C:12:GLU:N	2.30	0.64
1:A:217:ILE:CD1	1:A:234:LEU:HD13	2.27	0.64
2:C:9:VAL:HG12	2:C:13:TYR:CE2	2.34	0.63
1:A:480:TYR:CE1	1:A:484:LEU:HD22	2.34	0.63
1:B:268:ARG:NH2	4:B:609:HOH:O	2.31	0.62
1:B:216:PRO:HG3	1:B:270:LYS:HD2	1.82	0.62
2:D:112:ARG:NH2	2:D:147:ASN:OD1	2.27	0.62
1:B:450[A]:ARG:HE	1:B:450[A]:ARG:CA	2.12	0.62
1:A:214:LYS:HG2	1:A:233:HIS:CD2	2.35	0.61
1:A:483[A]:MET:HG3	1:A:484:LEU:N	2.15	0.61
1:B:286:TRP:HA	1:B:289[A]:VAL:CG1	2.30	0.60
1:A:509:THR:O	1:A:510:ARG:CB	2.39	0.60
2:C:32:VAL:CG1	2:C:134:LEU:HD11	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:26:GLN:HG2	2:C:142:ASP:HA	1.84	0.59
2:D:125:GLU:O	2:D:132:GLY:N	2.35	0.59
2:C:175:GLN:HE21	2:C:175:GLN:HA	1.68	0.59
1:B:192:THR:H	1:B:475:GLN:HE22	1.48	0.59
2:C:9:VAL:O	2:C:10:GLU:C	2.40	0.59
1:B:463:LEU:HD12	1:B:463:LEU:H	1.68	0.58
2:D:45:ILE:HD11	2:D:174:LEU:CD1	2.34	0.58
1:A:394:LEU:HD22	1:A:405:LEU:HD12	1.86	0.57
2:C:24:GLU:OE1	2:C:24:GLU:CA	2.51	0.57
1:B:265:GLU:CD	1:B:268:ARG:NH1	2.56	0.57
2:C:64:VAL:HG11	2:C:68:LYS:HA	1.87	0.56
1:A:216:PRO:HG3	1:A:270:LYS:HG3	1.87	0.56
2:C:19:ARG:CG	2:C:19:ARG:NH1	2.57	0.56
1:B:439:ASN:C	1:B:439:ASN:HD22	2.08	0.56
1:B:450[A]:ARG:HE	1:B:450[A]:ARG:HA	1.70	0.55
1:A:418:MET:CE	4:A:722:HOH:O	2.48	0.55
1:B:217:ILE:HG13	1:B:221:MET:HG3	1.89	0.55
1:A:217:ILE:HD11	1:A:234:LEU:HD13	1.89	0.54
1:A:310:VAL:HG13	4:A:629:HOH:O	2.07	0.54
1:A:446:ILE:O	1:A:450:ARG:HG2	2.08	0.54
2:C:16:LYS:HE3	2:C:17:HIS:CE1	2.36	0.54
2:C:9:VAL:N	2:C:12:GLU:OE1	2.41	0.54
1:B:439:ASN:ND2	1:B:442:GLU:H	2.06	0.53
2:C:28:SER:HB2	2:C:140:VAL:HG22	1.91	0.53
1:A:439:ASN:ND2	1:A:442:GLU:H	2.07	0.52
1:A:457:LYS:NZ	4:A:685:HOH:O	2.42	0.52
2:C:26:GLN:OE1	2:C:142:ASP:OD1	2.28	0.52
2:C:31:LEU:HD11	2:C:157:GLU:HG2	1.90	0.52
2:D:86:THR:OG1	2:D:110:ASP:OD1	2.25	0.52
1:A:449:ARG:O	1:A:453:MET:HG3	2.10	0.52
1:A:449:ARG:HG2	1:A:453:MET:HE2	1.85	0.51
2:C:76:GLU:OE2	2:C:89:THR:OG1	2.15	0.51
2:D:31:LEU:HD23	2:D:161:GLN:HG2	1.92	0.51
2:C:114:LYS:HG2	2:C:115:ASN:HD22	1.74	0.51
1:B:258[A]:LEU:HD23	1:B:297:VAL:HG21	1.93	0.50
2:C:16:LYS:CE	2:C:17:HIS:HE2	2.10	0.50
2:C:106:ILE:HG21	2:C:111:HIS:NE2	2.25	0.50
2:C:105:ARG:NH2	4:C:238:HOH:O	2.44	0.50
1:A:352:PHE:CG	1:A:444:CYS:HB3	2.46	0.49
1:B:219:MET:HG2	1:B:285:GLN:NE2	2.27	0.49
2:C:49:PHE:CD1	2:C:104:ILE:HD11	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:PRO:HG2	1:A:219:MET:CE	2.42	0.49
2:D:127:ILE:N	2:D:130:LYS:O	2.46	0.49
1:A:215:LEU:HD22	1:A:286:TRP:HH2	1.77	0.49
1:B:250:VAL:CG2	1:B:325:VAL:HG22	2.42	0.49
1:A:422:ARG:HB2	1:B:367:ASP:HB2	1.95	0.48
1:B:324:THR:HA	1:B:404:TYR:CD1	2.48	0.48
2:D:106:ILE:CG2	2:D:111:HIS:CE1	2.91	0.48
1:A:217:ILE:HD12	1:A:234:LEU:HD13	1.95	0.47
1:A:214:LYS:CG	1:A:233:HIS:CE1	2.97	0.47
1:A:214:LYS:HG2	1:A:233:HIS:CG	2.49	0.47
1:B:267:GLU:O	1:B:270:LYS:HB2	2.15	0.47
1:B:192:THR:H	1:B:475:GLN:NE2	2.12	0.47
2:D:68:LYS:HD2	2:D:70:GLU:CD	2.35	0.47
1:A:214:LYS:CD	1:A:233:HIS:CE1	2.96	0.47
1:B:286:TRP:HA	1:B:289[A]:VAL:HG12	1.97	0.47
1:A:199:ARG:HG3	1:A:492:ASP:HA	1.97	0.47
1:A:428:ILE:HD13	1:A:443:VAL:HG12	1.97	0.47
1:B:323:GLU:HB2	1:B:403:ARG:HG2	1.96	0.47
1:A:258[B]:LEU:HD13	1:A:258[B]:LEU:C	2.35	0.47
1:B:182:TYR:O	1:B:231:LEU:HD11	2.15	0.46
1:B:301[A]:ILE:HD11	4:B:528:HOH:O	2.14	0.46
1:B:250:VAL:HG13	1:B:301[B]:ILE:HD13	1.98	0.46
2:C:150[A]:GLU:HG2	4:C:214:HOH:O	2.14	0.46
2:C:123:HIS:CD2	2:C:136:ILE:HD12	2.51	0.46
1:A:214:LYS:HG3	1:A:233:HIS:ND1	2.31	0.45
2:D:179:MET:O	2:D:180:GLU:HG2	2.17	0.45
2:C:16:LYS:HE2	2:C:17:HIS:CD2	2.49	0.45
1:B:352:PHE:CG	1:B:444:CYS:HB3	2.52	0.45
1:A:491:LYS:HG3	1:A:491:LYS:H	1.66	0.45
1:A:192[A]:THR:H	1:A:475:GLN:NE2	2.09	0.45
2:C:108:GLY:O	2:C:111:HIS:HE1	2.00	0.45
2:C:24:GLU:OE1	2:C:25:SER:N	2.47	0.44
1:A:418:MET:HE3	1:A:419:PRO:HD2	1.99	0.44
1:A:226:GLY:H	1:B:377[A]:ASN:ND2	2.15	0.44
2:D:45:ILE:HD11	2:D:174:LEU:HD11	1.99	0.44
1:A:222:GLY:HA2	1:A:282[B]:ARG:CZ	2.48	0.44
1:A:258[B]:LEU:HD23	1:A:297:VAL:HG21	1.99	0.44
2:C:90:GLU:HG2	2:C:106:ILE:HG12	2.00	0.44
1:A:192[A]:THR:HG21	1:A:206:PHE:CE1	2.52	0.44
1:A:226:GLY:H	1:B:377[A]:ASN:HD22	1.65	0.44
2:D:104:ILE:CG2	2:D:105:ARG:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:141:VAL:HG22	2:C:142:ASP:N	2.34	0.43
1:A:192[B]:THR:H	1:A:475:GLN:NE2	2.12	0.43
1:A:214:LYS:CG	1:A:233:HIS:CG	3.02	0.43
1:B:313:SER:HA	1:B:314:ASP:HA	1.59	0.43
2:C:9:VAL:HB	2:C:10:GLU:H	1.45	0.43
2:C:69:LEU:HD23	2:C:69:LEU:HA	1.76	0.43
2:C:16:LYS:HG3	2:C:17:HIS:N	2.34	0.42
1:B:216:PRO:HG3	1:B:270:LYS:CD	2.46	0.42
2:C:108:GLY:O	2:C:111:HIS:CE1	2.71	0.42
1:A:199:ARG:HD3	4:A:550:HOH:O	2.18	0.42
2:C:150[B]:GLU:H	2:C:150[B]:GLU:CD	2.21	0.42
1:A:219:MET:O	1:A:282[B]:ARG:HG2	2.19	0.42
2:C:115:ASN:HA	4:C:201:HOH:O	2.18	0.42
1:A:372:TYR:CE2	1:A:376:GLU:HG3	2.55	0.42
1:B:258[B]:LEU:C	1:B:258[B]:LEU:HD23	2.40	0.42
1:A:483[A]:MET:CG	1:A:484:LEU:N	2.80	0.42
2:C:152:THR:O	2:C:156:VAL:HG23	2.19	0.42
2:D:87:LYS:HB3	2:D:87:LYS:HE2	1.45	0.42
1:B:268:ARG:C	1:B:270:LYS:N	2.72	0.41
1:A:448:ARG:NH1	4:A:705:HOH:O	2.53	0.41
2:D:45:ILE:HD11	2:D:174:LEU:HD12	2.02	0.41
2:C:29:SER:HB3	2:C:139:PHE:CE2	2.54	0.41
1:A:193[A]:VAL:HG12	1:A:496:ILE:HB	2.03	0.41
1:A:492:ASP:OD1	1:A:493:ASN:N	2.53	0.41
1:B:474:CYS:SG	1:B:500:ASP:HB2	2.61	0.41
1:B:258[A]:LEU:CD2	1:B:297:VAL:HG21	2.50	0.41
1:A:180:SER:O	1:A:184:LEU:HD22	2.20	0.41
2:C:104:ILE:HG23	2:C:105:ARG:N	2.36	0.41
1:A:406:LYS:HE3	4:A:713:HOH:O	2.20	0.41
1:B:483:MET:HG3	1:B:484:LEU:N	2.36	0.41
2:C:175:GLN:NE2	2:C:175:GLN:HA	2.34	0.41
1:A:330:VAL:HG13	1:A:330:VAL:O	2.21	0.41
2:C:180:GLU:HA	2:C:180:GLU:OE2	2.22	0.40
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.82	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:23:VAL:N	2:D:26:GLN:NE2[1_556]	2.09	0.11

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	332/340 (98%)	328 (99%)	4 (1%)	0	100	100
1	B	317/340 (93%)	308 (97%)	9 (3%)	0	100	100
2	C	171/183 (93%)	164 (96%)	6 (4%)	1 (1%)	30	24
2	D	152/183 (83%)	149 (98%)	3 (2%)	0	100	100
All	All	972/1046 (93%)	949 (98%)	22 (2%)	1 (0%)	56	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	10	GLU

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	282/285 (99%)	252 (89%)	30 (11%)	8	4
1	B	271/285 (95%)	248 (92%)	23 (8%)	13	9
2	C	158/167 (95%)	141 (89%)	17 (11%)	8	4
2	D	144/167 (86%)	129 (90%)	15 (10%)	9	5
All	All	855/904 (95%)	770 (90%)	85 (10%)	11	6

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	LEU
1	A	199	ARG
1	A	214	LYS
1	A	228	SER
1	A	267	GLU
1	A	276	ARG
1	A	282[A]	ARG
1	A	282[B]	ARG
1	A	287	ASP
1	A	288	LYS
1	A	293	CYS
1	A	304	LYS
1	A	320	VAL
1	A	333	LEU
1	A	355	LYS
1	A	394	LEU
1	A	404	TYR
1	A	409	VAL
1	A	422	ARG
1	A	434	LEU
1	A	439	ASN
1	A	448	ARG
1	A	449	ARG
1	A	457	LYS
1	A	463	LEU
1	A	466	ARG
1	A	483[A]	MET
1	A	483[B]	MET
1	A	491	LYS
1	A	510	ARG
1	B	214	LYS
1	B	230	SER
1	B	231	LEU
1	B	270	LYS
1	B	271	ASP
1	B	289[A]	VAL
1	B	289[B]	VAL
1	B	293	CYS
1	B	295	LEU
1	B	301[A]	ILE
1	B	301[B]	ILE
1	B	312	SER
1	B	325	VAL

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Mol	Chain	Res	Type
1	B	336[A]	SER
1	B	336[B]	SER
1	B	409	VAL
1	B	434	LEU
1	B	439	ASN
1	B	450[A]	ARG
1	B	450[B]	ARG
1	B	456	LYS
1	B	483	MET
1	B	506	LYS
2	C	9	VAL
2	C	10	GLU
2	C	14	ILE
2	C	16	LYS
2	C	19	ARG
2	C	20	HIS
2	C	23	VAL
2	C	24	GLU
2	C	25	SER
2	C	53	GLN
2	C	83	LEU
2	C	104	ILE
2	C	130	LYS
2	C	150[A]	GLU
2	C	150[B]	GLU
2	C	175	GLN
2	C	178	SER
2	D	53	GLN
2	D	61	ARG
2	D	65	GLN
2	D	70	GLU
2	D	76	GLU
2	D	83	LEU
2	D	87	LYS
2	D	104	ILE
2	D	126	THR
2	D	127	ILE
2	D	140	VAL
2	D	145	GLU
2	D	154	PHE
2	D	162	SER
2	D	175	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	343	ASN
1	A	384	GLN
1	A	439	ASN
1	A	475	GLN
1	B	285	GLN
1	B	343	ASN
1	B	439	ASN
1	B	458	ASN
1	B	475	GLN
2	C	26	GLN
2	C	40	HIS
2	C	53	GLN
2	C	111	HIS
2	C	115	ASN
2	C	175	GLN
2	D	53	GLN
2	D	175	GLN

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	328/340 (96%)	-0.12	9 (2%) 58 65	13, 24, 63, 135	0
1	B	314/340 (92%)	0.15	17 (5%) 29 37	15, 28, 66, 152	0
2	C	172/183 (93%)	0.35	18 (10%) 8 11	20, 36, 100, 156	0
2	D	158/183 (86%)	0.20	10 (6%) 23 30	19, 37, 98, 151	0
All	All	972/1046 (92%)	0.10	54 (5%) 28 36	13, 31, 79, 156	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	THR	10.2
2	C	23	VAL	10.1
2	D	15	LYS	7.1
2	D	16	LYS	5.6
2	C	24	GLU	4.9
1	B	230	SER	4.7
2	C	9	VAL	4.6
2	C	19	ARG	4.5
1	A	228	SER	4.5
1	B	279	GLY	4.4
1	B	231	LEU	4.4
2	D	18	HIS	4.3
1	A	463	LEU	3.7
1	A	184	LEU	3.6
1	B	312	SER	3.6
2	D	127	ILE	3.5
2	D	67	LYS	3.4
1	A	508	LYS	3.4
1	B	311	GLY	3.3
2	C	21	GLU	3.2
2	C	22	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	25	SER	3.1
1	B	271	ASP	3.1
2	C	16	LYS	3.1
2	D	131	THR	3.0
2	C	67	LYS	3.0
2	D	130	LYS	3.0
1	B	316	VAL	3.0
1	A	510	ARG	3.0
2	D	176	ALA	2.9
1	B	313	SER	2.9
2	C	15	LYS	2.8
1	B	506	LYS	2.8
2	D	126	THR	2.7
1	B	463	LEU	2.6
1	B	185	ASP	2.6
1	A	464	ALA	2.5
2	C	12	GLU	2.5
2	C	66	GLY	2.5
2	C	10	GLU	2.4
2	C	68	LYS	2.4
2	C	11	SER	2.4
1	B	462	PRO	2.3
2	C	26	GLN	2.2
1	B	309	VAL	2.2
2	D	17	HIS	2.2
1	A	185	ASP	2.2
1	B	317	LEU	2.2
1	B	200	SER	2.2
2	C	65	GLN	2.2
1	A	227	MET	2.2
1	A	509	THR	2.1
2	C	13	TYR	2.1
1	B	331	VAL	2.1

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 [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(\AA^2)	Q<0.9
3	MG	B	512	1/1	0.99	0.15	4.07	19,19,19,19	0
3	MG	A	512	1/1	0.99	0.13	1.94	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.