



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:05 PM GMT

PDB ID : 3SJB
Title : Crystal structure of *S. cerevisiae* Get3 in the open state in complex with Get1 cytosolic domain
Authors : Reitz, S.; Wild, K.; Sinning, I.
Deposited on : 2011-06-21
Resolution : 3.30 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

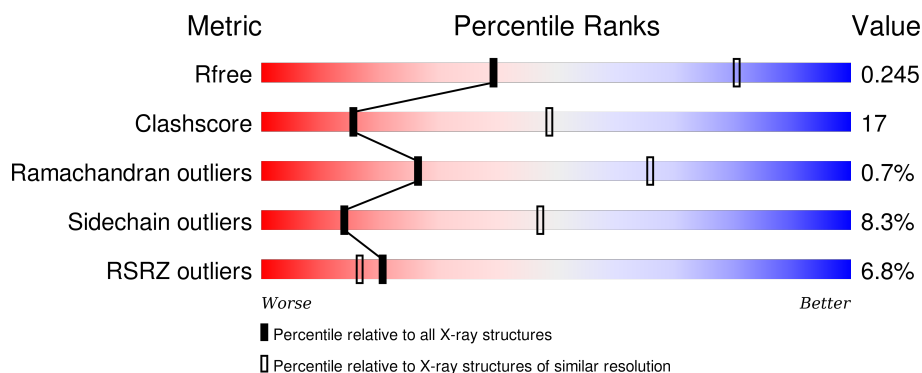
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	362	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>26%</div> <div>•</div> <div>20%</div> </div> </div>
1	B	362	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>28%</div> <div>•</div> <div>17%</div> </div> </div>
2	C	93	<div> <div>8%</div> <div> <div></div> <div>49%</div> <div>17%</div> <div>•</div> <div>32%</div> </div> </div>
2	D	93	<div> <div>10%</div> <div> <div></div> <div>48%</div> <div>27%</div> <div>•</div> <div>23%</div> </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	PO4	A	364	-	-	-	X
3	PO4	B	363	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5823 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2280	1437	380	447	16			
1	B	302	Total	C	N	O	S	0	0	0
			2384	1503	396	468	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	LEU	-	EXPRESSION TAG	UNP Q12154
A	356	GLU	-	EXPRESSION TAG	UNP Q12154
A	357	HIS	-	EXPRESSION TAG	UNP Q12154
A	358	HIS	-	EXPRESSION TAG	UNP Q12154
A	359	HIS	-	EXPRESSION TAG	UNP Q12154
A	360	HIS	-	EXPRESSION TAG	UNP Q12154
A	361	HIS	-	EXPRESSION TAG	UNP Q12154
A	362	HIS	-	EXPRESSION TAG	UNP Q12154
B	355	LEU	-	EXPRESSION TAG	UNP Q12154
B	356	GLU	-	EXPRESSION TAG	UNP Q12154
B	357	HIS	-	EXPRESSION TAG	UNP Q12154
B	358	HIS	-	EXPRESSION TAG	UNP Q12154
B	359	HIS	-	EXPRESSION TAG	UNP Q12154
B	360	HIS	-	EXPRESSION TAG	UNP Q12154
B	361	HIS	-	EXPRESSION TAG	UNP Q12154
B	362	HIS	-	EXPRESSION TAG	UNP Q12154

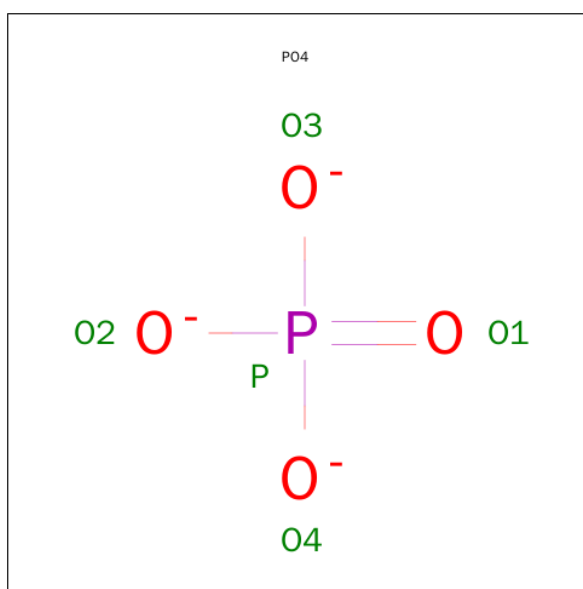
- Molecule 2 is a protein called Golgi to ER traffic protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	63	Total	C	N	O	0	0	0
			528	328	96	104			
2	D	72	Total	C	N	O	0	0	0
			610	379	115	116			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	18	MET	-	EXPRESSION TAG	UNP P53192
C	104	GLU	-	EXPRESSION TAG	UNP P53192
C	105	HIS	-	EXPRESSION TAG	UNP P53192
C	106	HIS	-	EXPRESSION TAG	UNP P53192
C	107	HIS	-	EXPRESSION TAG	UNP P53192
C	108	HIS	-	EXPRESSION TAG	UNP P53192
C	109	HIS	-	EXPRESSION TAG	UNP P53192
C	110	HIS	-	EXPRESSION TAG	UNP P53192
D	18	MET	-	EXPRESSION TAG	UNP P53192
D	104	GLU	-	EXPRESSION TAG	UNP P53192
D	105	HIS	-	EXPRESSION TAG	UNP P53192
D	106	HIS	-	EXPRESSION TAG	UNP P53192
D	107	HIS	-	EXPRESSION TAG	UNP P53192
D	108	HIS	-	EXPRESSION TAG	UNP P53192
D	109	HIS	-	EXPRESSION TAG	UNP P53192
D	110	HIS	-	EXPRESSION TAG	UNP P53192

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0

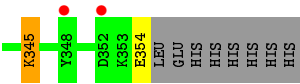
Continued on next page...

Continued from previous page...

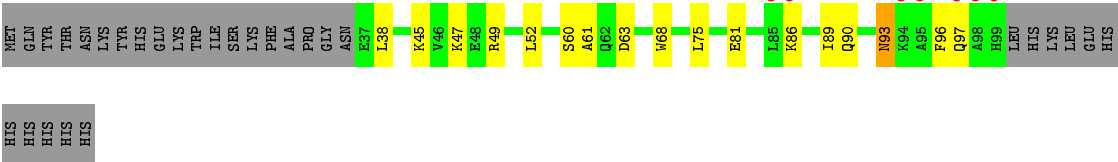
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

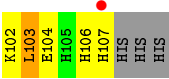
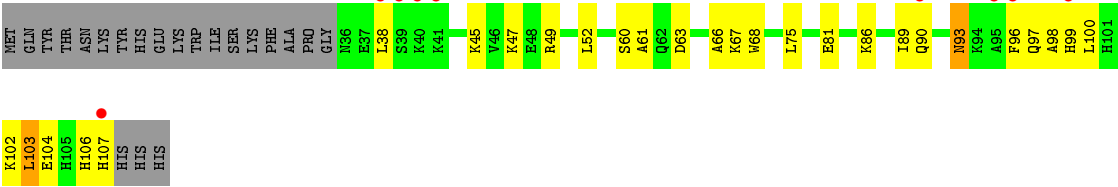
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		



• Molecule 2: Golgi to ER traffic protein 1



• Molecule 2: Golgi to ER traffic protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	112.90Å 112.90Å 310.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.89 – 3.30 48.89 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.89-3.30) 99.6 (48.89-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, R_{free}	0.195 , 0.243 0.192 , 0.245	Depositor DCC
R_{free} test set	940 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	110.7	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 103.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 18399 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5823	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: ZN, PO4

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	0.47	0/2318	0.63	0/3125
1	B	0.45	0/2423	0.61	0/3268
2	C	0.39	0/535	0.47	0/713
2	D	0.35	0/621	0.48	0/829
All	All	0.45	0/5897	0.60	0/7935

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 [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	2280	0	2246	82	0
1	B	2384	0	2357	91	0
2	C	528	0	523	10	0
2	D	610	0	598	19	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	1	0	0	0	0
All	All	5823	0	5724	198	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 17.

All (198) 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:20:TRP:HB2	1:B:236:THR:HB	1.45	0.98
1:A:20:TRP:HB2	1:A:236:THR:HB	1.47	0.96
1:A:29:VAL:HG12	1:A:243:ILE:HD13	1.44	0.96
1:B:29:VAL:HG12	1:B:243:ILE:HD13	1.44	0.95
1:A:72:LYS:HD3	1:A:72:LYS:N	1.87	0.87
1:A:292:TRP:NE1	1:A:296:LYS:HE2	1.89	0.87
1:B:72:LYS:N	1:B:72:LYS:HD3	1.89	0.85
1:B:292:TRP:NE1	1:B:296:LYS:HE2	1.92	0.84
1:A:254:ARG:HG2	1:A:254:ARG:HH11	1.43	0.83
1:B:180:PRO:HD3	1:B:223:VAL:HG11	1.59	0.82
1:B:254:ARG:HG2	1:B:254:ARG:HH11	1.46	0.81
1:B:61:ASN:H	1:B:61:ASN:HD22	1.31	0.79
1:A:135:GLY:HA2	1:A:138:GLU:HB2	1.65	0.78
1:A:8:ASN:HA	1:A:312:VAL:HG13	1.66	0.77
1:B:8:ASN:HA	1:B:312:VAL:HG13	1.66	0.77
2:D:86:LYS:O	2:D:90:GLN:HG2	1.85	0.77
1:B:225:THR:O	1:B:228:GLN:HG3	1.86	0.76
2:C:86:LYS:O	2:C:90:GLN:HG2	1.85	0.76
1:B:15:SER:OG	1:B:18:HIS:HD2	1.70	0.75
1:A:61:ASN:H	1:A:61:ASN:HD22	1.32	0.75
1:B:135:GLY:HA2	1:B:138:GLU:HB2	1.70	0.74
2:D:38:LEU:HD23	2:D:89:ILE:HG13	1.70	0.74
1:B:153:GLU:HG2	1:B:159:THR:HA	1.70	0.74
2:C:38:LEU:HD23	2:C:89:ILE:HG13	1.69	0.74
1:A:225:THR:O	1:A:228:GLN:HG3	1.87	0.73
1:B:179:LEU:N	1:B:180:PRO:HD2	2.04	0.73
1:B:54:ILE:HG13	1:B:86:MET:HG3	1.72	0.72
1:A:153:GLU:HG2	1:A:159:THR:HA	1.69	0.72
2:D:102:LYS:O	2:D:106:HIS:HB2	1.91	0.71
1:A:15:SER:OG	1:A:18:HIS:HD2	1.74	0.71
1:B:136:ILE:HD13	1:B:179:LEU:HD21	1.72	0.70
1:A:54:ILE:HG13	1:A:86:MET:HG3	1.73	0.70
1:B:231:THR:O	1:B:233:PRO:HD3	1.92	0.68
1:A:318:ALA:HB2	1:B:287:ARG:HG2	1.75	0.68
1:A:72:LYS:HD3	1:A:72:LYS:H	1.57	0.68
1:A:231:THR:O	1:A:233:PRO:HD3	1.94	0.67
1:B:20:TRP:HB2	1:B:236:THR:CB	2.24	0.67
2:D:102:LYS:O	2:D:106:HIS:CB	2.43	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LEU:O	1:B:13:ILE:HG13	1.94	0.67
1:A:249:LEU:HD21	1:A:302:ILE:HD11	1.77	0.66
1:A:305:LEU:HD13	2:D:66:ALA:HA	1.78	0.65
1:B:72:LYS:H	1:B:72:LYS:HD3	1.61	0.65
1:A:305:LEU:HD23	1:A:306:TYR:CE2	2.32	0.65
1:A:292:TRP:HE1	1:A:296:LYS:HE2	1.61	0.64
1:B:285:CYS:SG	1:B:287:ARG:HB2	2.37	0.64
1:B:61:ASN:ND2	1:B:61:ASN:H	1.94	0.63
1:A:61:ASN:H	1:A:61:ASN:ND2	1.96	0.63
1:A:254:ARG:HH11	1:A:254:ARG:CG	2.10	0.63
1:A:287:ARG:HG2	1:B:318:ALA:HB2	1.78	0.63
1:A:224:GLU:HG2	1:A:227:ARG:NH2	2.12	0.63
1:B:329:LYS:O	1:B:332:GLN:HG2	1.98	0.63
1:B:254:ARG:CG	1:B:254:ARG:HH11	2.12	0.63
1:A:20:TRP:HB2	1:A:236:THR:CB	2.25	0.62
1:A:285:CYS:SG	1:A:288:CYS:N	2.70	0.62
1:B:224:GLU:HG2	1:B:227:ARG:NH2	2.14	0.62
1:A:9:LEU:O	1:A:13:ILE:HG13	2.00	0.62
2:C:49:ARG:HD2	2:C:75:LEU:HD22	1.81	0.61
1:A:285:CYS:SG	1:A:287:ARG:HB2	2.41	0.60
1:B:185:LYS:O	1:B:188:GLU:HG2	2.01	0.60
2:C:61:ALA:HB2	2:C:68:TRP:CE2	2.36	0.60
1:A:329:LYS:O	1:A:332:GLN:HG2	2.02	0.60
1:A:143:MET:O	1:A:147:LYS:HG3	2.01	0.60
1:B:180:PRO:HG2	1:B:227:ARG:NH1	2.18	0.59
2:D:49:ARG:HD2	2:D:75:LEU:HD22	1.82	0.59
1:B:126:LEU:O	1:B:130:THR:HB	2.01	0.59
1:B:96:ASP:O	1:B:100:MET:HG2	2.03	0.59
1:B:305:LEU:HD23	1:B:306:TYR:CE2	2.38	0.59
1:A:320:GLU:HA	1:A:320:GLU:OE1	2.02	0.59
1:A:133:ILE:HB	1:A:136:ILE:HG13	1.85	0.59
1:A:172:HIS:HB2	1:A:175:ARG:HH11	1.69	0.58
1:B:172:HIS:HB2	1:B:175:ARG:HH11	1.69	0.58
1:B:249:LEU:HD21	1:B:302:ILE:HD11	1.84	0.58
2:C:60:SER:HB3	2:C:63:ASP:HB2	1.84	0.57
1:B:232:ASP:HB3	1:B:235:LEU:HB2	1.86	0.57
1:B:320:GLU:OE1	1:B:320:GLU:HA	2.04	0.56
1:B:285:CYS:SG	1:B:288:CYS:N	2.73	0.56
1:B:143:MET:O	1:B:147:LYS:HG3	2.05	0.56
1:B:133:ILE:HB	1:B:136:ILE:HG13	1.87	0.56
1:A:61:ASN:N	1:A:61:ASN:HD22	1.96	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HA	1:A:51:PHE:CE2	2.40	0.56
1:B:292:TRP:HE1	1:B:296:LYS:HE2	1.66	0.56
2:D:104:GLU:O	2:D:107:HIS:HB2	2.05	0.56
1:B:43:ALA:HA	1:B:51:PHE:CE2	2.40	0.56
1:A:61:ASN:ND2	1:A:61:ASN:N	2.52	0.55
2:C:52:LEU:HD23	2:C:75:LEU:HD23	1.89	0.54
2:D:60:SER:HB3	2:D:63:ASP:HB2	1.88	0.54
1:B:61:ASN:HD22	1:B:61:ASN:N	1.95	0.54
2:C:45:LYS:HE3	2:C:81:GLU:OE1	2.08	0.54
1:A:74:ALA:HB2	1:A:86:MET:CE	2.37	0.54
1:A:232:ASP:HB3	1:A:235:LEU:HB2	1.89	0.54
2:D:61:ALA:HB2	2:D:68:TRP:CE2	2.43	0.54
1:A:39:ALA:HA	1:A:164:ILE:CD1	2.37	0.54
1:B:7:PRO:HG2	1:B:337:GLU:OE2	2.08	0.54
1:B:20:TRP:CB	1:B:236:THR:HB	2.31	0.53
1:B:39:ALA:HA	1:B:164:ILE:CD1	2.38	0.53
1:B:39:ALA:HA	1:B:164:ILE:HD13	1.90	0.53
1:B:136:ILE:O	1:B:140:LEU:HD22	2.08	0.53
1:B:320:GLU:HG2	1:B:322:ARG:CZ	2.38	0.53
1:A:30:GLY:HA3	1:A:272:ASN:HD22	1.73	0.53
1:B:255:LEU:HD12	1:B:255:LEU:O	2.09	0.53
2:D:45:LYS:HE3	2:D:81:GLU:OE1	2.09	0.52
1:B:180:PRO:HD3	1:B:223:VAL:CG1	2.34	0.52
1:A:320:GLU:HG2	1:A:322:ARG:CZ	2.39	0.52
1:B:61:ASN:ND2	1:B:61:ASN:N	2.50	0.52
1:B:282:GLU:O	1:B:284:ASN:N	2.42	0.52
1:A:39:ALA:HA	1:A:164:ILE:HD13	1.91	0.52
1:A:282:GLU:O	1:A:284:ASN:N	2.42	0.52
1:A:229:GLN:O	1:A:236:THR:HG23	2.10	0.51
1:B:229:GLN:O	1:B:236:THR:HG23	2.10	0.51
1:A:255:LEU:HD12	1:A:255:LEU:O	2.10	0.51
1:A:130:THR:HG22	1:A:131:GLY:N	2.25	0.51
1:B:130:THR:HG22	1:B:131:GLY:N	2.26	0.51
1:B:134:PRO:HB3	1:B:175:ARG:HE	1.75	0.50
1:A:231:THR:HG22	1:A:231:THR:O	2.11	0.50
1:B:29:VAL:HG12	1:B:243:ILE:CD1	2.30	0.50
1:B:180:PRO:HB3	1:B:224:GLU:HG3	1.93	0.50
1:A:55:SER:HB2	1:A:166:ASP:HB3	1.94	0.50
1:B:231:THR:O	1:B:231:THR:HG22	2.12	0.50
1:B:306:TYR:O	1:B:309:PHE:HB2	2.11	0.50
1:A:282:GLU:C	1:A:284:ASN:N	2.65	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLY:HA3	1:B:272:ASN:HD22	1.76	0.50
1:B:74:ALA:HB2	1:B:86:MET:CE	2.41	0.50
1:B:5:VAL:HG12	1:B:310:HIS:CE1	2.46	0.50
1:B:282:GLU:C	1:B:284:ASN:N	2.64	0.50
1:B:180:PRO:CG	1:B:227:ARG:NH1	2.75	0.49
1:A:7:PRO:HG2	1:A:337:GLU:OE2	2.13	0.49
1:A:306:TYR:O	1:A:309:PHE:HB2	2.13	0.49
1:A:136:ILE:O	1:A:140:LEU:HD22	2.14	0.48
1:A:5:VAL:HG12	1:A:310:HIS:CE1	2.48	0.48
1:B:55:SER:HB2	1:B:166:ASP:HB3	1.96	0.48
2:D:52:LEU:HD23	2:D:75:LEU:HD23	1.94	0.48
1:A:254:ARG:NH1	1:A:254:ARG:CG	2.75	0.48
1:B:74:ALA:HB2	1:B:86:MET:HE2	1.96	0.48
1:A:144:GLU:OE2	1:A:147:LYS:HD2	2.14	0.48
2:D:102:LYS:O	2:D:106:HIS:HB3	2.12	0.47
1:B:5:VAL:HG21	1:B:308:ASP:HA	1.96	0.47
1:B:282:GLU:O	1:B:283:HIS:C	2.53	0.47
2:C:52:LEU:HD23	2:C:75:LEU:CD2	2.44	0.47
1:A:273:GLN:HG2	1:A:316:LEU:HD13	1.97	0.47
1:B:52:LEU:HD12	1:B:84:SER:O	2.15	0.47
1:A:249:LEU:CD2	1:A:302:ILE:HD11	2.44	0.47
1:A:282:GLU:O	1:A:283:HIS:C	2.53	0.47
1:A:20:TRP:CB	1:A:236:THR:HB	2.32	0.46
1:A:139:ALA:O	1:A:143:MET:HG2	2.15	0.46
1:B:178:GLN:C	1:B:180:PRO:HD2	2.36	0.45
2:D:52:LEU:HD23	2:D:75:LEU:CD2	2.45	0.45
1:B:179:LEU:N	1:B:180:PRO:CD	2.76	0.45
1:A:74:ALA:HB2	1:A:86:MET:HE3	1.98	0.45
1:B:30:GLY:HA3	1:B:272:ASN:ND2	2.31	0.45
1:A:5:VAL:HG21	1:A:308:ASP:HA	1.98	0.45
1:B:95:LYS:HE2	1:B:99:ASP:OD1	2.17	0.45
1:B:254:ARG:NH1	1:B:254:ARG:CG	2.76	0.45
2:D:47:LYS:HD2	2:D:47:LYS:C	2.38	0.44
1:B:144:GLU:OE2	1:B:147:LYS:HD2	2.17	0.44
1:A:139:ALA:HB2	1:A:176:PHE:HB2	1.97	0.44
1:A:30:GLY:HA3	1:A:272:ASN:ND2	2.30	0.44
2:D:99:HIS:O	2:D:103:LEU:HG	2.17	0.44
1:A:274:LEU:HD22	1:A:299:LEU:HD11	1.99	0.44
1:B:139:ALA:O	1:B:143:MET:HG2	2.18	0.43
1:B:304:GLU:O	1:B:304:GLU:HG3	2.17	0.43
1:B:230:PHE:HD1	1:B:236:THR:HG21	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASN:O	1:A:225:THR:HB	2.18	0.43
2:D:93:ASN:O	2:D:97:GLN:HB2	2.17	0.43
1:B:13:ILE:HD13	1:B:41:GLN:HB3	2.00	0.43
1:A:134:PRO:HB3	1:A:175:ARG:HE	1.83	0.43
2:C:47:LYS:C	2:C:47:LYS:HD2	2.38	0.43
2:D:67:LYS:HB2	2:D:67:LYS:HE3	1.78	0.42
1:A:318:ALA:HB2	1:B:287:ARG:CG	2.48	0.42
1:B:235:LEU:HA	1:B:235:LEU:HD23	1.87	0.42
1:A:149:ILE:O	1:A:152:GLN:HB2	2.20	0.42
2:C:93:ASN:O	2:C:97:GLN:HB2	2.20	0.42
1:A:280:ASP:O	1:A:283:HIS:ND1	2.53	0.42
1:A:230:PHE:HD1	1:A:236:THR:HG21	1.84	0.42
1:A:296:LYS:HB2	1:A:296:LYS:HE3	1.75	0.42
1:A:74:ALA:HB2	1:A:86:MET:HE2	2.01	0.42
1:A:227:ARG:HE	1:A:227:ARG:HB3	1.58	0.42
1:A:246:PHE:C	1:A:246:PHE:CD1	2.93	0.42
1:A:339:ASN:HA	1:A:340:PRO:HD3	1.86	0.41
1:B:345:LYS:HB3	1:B:345:LYS:HE3	1.82	0.41
1:A:13:ILE:HD13	1:A:41:GLN:HB3	2.01	0.41
1:B:139:ALA:HB2	1:B:176:PHE:HB2	2.01	0.41
1:A:133:ILE:HA	1:A:134:PRO:HD3	1.73	0.41
1:B:149:ILE:O	1:B:152:GLN:HB2	2.19	0.41
1:B:262:TYR:O	1:B:263:ASP:HB2	2.20	0.41
1:A:52:LEU:HD12	1:A:84:SER:O	2.20	0.41
1:A:324:LEU:HA	1:A:324:LEU:HD12	1.83	0.41
1:A:253:GLU:O	1:A:254:ARG:C	2.59	0.41
1:B:273:GLN:HG2	1:B:316:LEU:HD13	2.03	0.41
2:D:100:LEU:HD23	2:D:100:LEU:C	2.41	0.41
1:B:296:LYS:HB2	1:B:296:LYS:HE3	1.78	0.41
1:A:255:LEU:HD12	1:A:255:LEU:C	2.41	0.41
1:B:133:ILE:HA	1:B:134:PRO:HD3	1.72	0.40
1:B:339:ASN:OD1	1:B:339:ASN:C	2.60	0.40
1:B:255:LEU:HD12	1:B:255:LEU:C	2.41	0.40
1:B:280:ASP:O	1:B:283:HIS:ND1	2.53	0.40
2:D:98:ALA:O	2:D:102:LYS:HB2	2.21	0.40
1:B:43:ALA:HA	1:B:51:PHE:CD2	2.56	0.40
1:A:56:THR:O	1:A:57:ASP:C	2.60	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	282/362 (78%)	254 (90%)	26 (9%)	2 (1%)	26	66
1	B	296/362 (82%)	272 (92%)	22 (7%)	2 (1%)	26	66
2	C	61/93 (66%)	57 (93%)	4 (7%)	0	100	100
2	D	70/93 (75%)	66 (94%)	3 (4%)	1 (1%)	14	50
All	All	709/910 (78%)	649 (92%)	55 (8%)	5 (1%)	26	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	283	HIS
1	B	60	HIS
1	B	283	HIS
2	D	103	LEU

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	257/317 (81%)	233 (91%)	24 (9%)	11	40
1	B	269/317 (85%)	243 (90%)	26 (10%)	10	38
2	C	58/86 (67%)	56 (97%)	2 (3%)	44	77
2	D	67/86 (78%)	65 (97%)	2 (3%)	48	79
All	All	651/806 (81%)	597 (92%)	54 (8%)	14	47

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	64	ASP
1	A	72	LYS
1	A	75	ARG
1	A	80	MET
1	A	81	ASN
1	A	84	SER
1	A	140	LEU
1	A	144	GLU
1	A	236	THR
1	A	243	ILE
1	A	247	LEU
1	A	254	ARG
1	A	255	LEU
1	A	264	MET
1	A	268	SER
1	A	285	CYS
1	A	289	GLN
1	A	291	ARG
1	A	294	MET
1	A	311	VAL
1	A	312	VAL
1	A	345	LYS
1	A	354	GLU
1	B	61	ASN
1	B	64	ASP
1	B	72	LYS
1	B	75	ARG
1	B	80	MET
1	B	81	ASN
1	B	84	SER
1	B	140	LEU
1	B	144	GLU
1	B	186	LEU
1	B	187	LEU
1	B	236	THR
1	B	243	ILE
1	B	247	LEU
1	B	254	ARG
1	B	255	LEU
1	B	264	MET
1	B	268	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	285	CYS
1	B	289	GLN
1	B	291	ARG
1	B	294	MET
1	B	311	VAL
1	B	312	VAL
1	B	345	LYS
1	B	354	GLU
2	C	93	ASN
2	C	96	PHE
2	D	93	ASN
2	D	96	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	41	GLN
1	A	61	ASN
1	A	279	ASN
1	A	281	GLN
1	A	289	GLN
1	A	326	ASN
1	B	18	HIS
1	B	61	ASN
1	B	217	ASN
1	B	279	ASN
1	B	281	GLN
1	B	289	GLN
1	B	326	ASN
2	D	36	ASN
2	D	62	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
3	PO4	A	363	-	4,4,4	0.41	0	6,6,6	0.30	0
3	PO4	A	364	-	4,4,4	0.44	0	6,6,6	0.28	0
3	PO4	B	363	-	4,4,4	0.39	0	6,6,6	0.27	0
3	PO4	B	364	-	4,4,4	0.38	0	6,6,6	0.28	0

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
3	PO4	A	363	-	-	0/0/0/0	0/0/0/0
3	PO4	A	364	-	-	0/0/0/0	0/0/0/0
3	PO4	B	363	-	-	0/0/0/0	0/0/0/0
3	PO4	B	364	-	-	0/0/0/0	0/0/0/0

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 [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 ⓘ

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	288/362 (79%)	0.16	14 (4%) 33 27	65, 109, 218, 258	0
1	B	302/362 (83%)	0.26	19 (6%) 23 19	64, 111, 223, 268	0
2	C	63/93 (67%)	0.38	7 (11%) 7 6	86, 129, 202, 219	0
2	D	72/93 (77%)	0.43	9 (12%) 5 4	87, 139, 229, 256	0
All	All	725/910 (79%)	0.25	49 (6%) 20 17	64, 114, 221, 268	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	ASP	6.2
1	B	128	ASP	6.2
1	B	223	VAL	5.8
1	B	219	LEU	5.2
1	B	184	SER	4.8
1	A	129	LEU	4.6
2	D	96	PHE	4.4
1	B	183	LEU	4.4
1	A	283	HIS	4.3
2	C	99	HIS	4.0
2	D	90	GLN	4.0
1	A	128	ASP	3.9
1	A	127	ALA	3.8
2	D	95	ALA	3.8
2	D	107	HIS	3.7
1	A	214	GLY	3.7
1	B	284	ASN	3.7
1	B	182	THR	3.7
1	B	187	LEU	3.6
2	C	98	ALA	3.6
1	A	284	ASN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	98	ASN	3.4
1	B	283	HIS	3.4
1	A	130	THR	3.2
1	A	280	ASP	3.1
2	C	86	LYS	3.0
2	C	97	GLN	3.0
1	A	348	TYR	2.9
2	C	94	LYS	2.8
2	C	95	ALA	2.8
1	A	354	GLU	2.7
1	B	281	GLN	2.7
2	D	99	HIS	2.6
2	D	38	LEU	2.6
1	B	129	LEU	2.5
2	D	41	LYS	2.5
2	D	39	SER	2.5
1	B	94	LEU	2.5
1	B	352	ASP	2.4
1	A	217	ASN	2.3
1	A	133	ILE	2.3
1	A	215	LYS	2.3
1	B	97	MET	2.2
1	B	100	MET	2.2
1	B	348	TYR	2.1
2	D	40	LYS	2.1
1	B	101	ALA	2.1
1	A	149	ILE	2.0
2	C	85	LEU	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
3	PO4	A	364	5/5	0.85	0.41	5.60	140,151,158,175	0
3	PO4	B	363	5/5	0.93	0.37	3.38	166,169,178,184	0
3	PO4	A	363	5/5	0.93	0.35	1.58	150,152,160,172	0
3	PO4	B	364	5/5	0.84	0.28	1.02	122,143,153,179	0
4	ZN	A	365	1/1	1.00	0.10	-	106,106,106,106	0

6.5 Other polymers

There are no such residues in this entry.