Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:09 am BST

PDB ID	:	3ZS8
Title	:	S. cerevisiae Get3 complexed with a cytosolic Get1 fragment
Authors	:	Mariappan, M.; Mateja, A.; Dobosz, M.; Bove, E.; Hegde, R.S.; Keenan, R.J.
Deposited on	:	2011-06-24
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

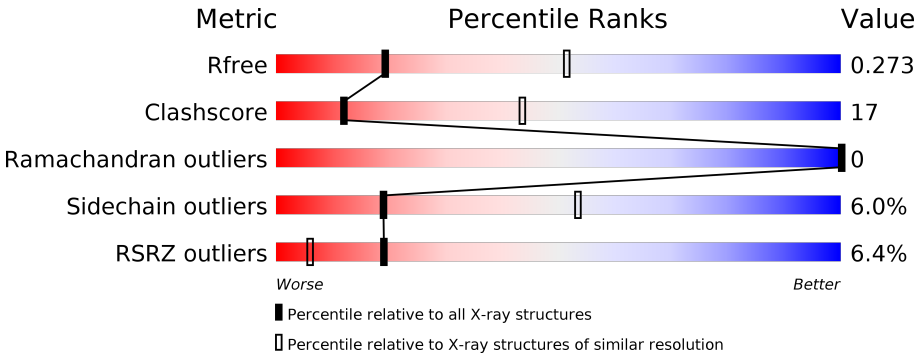
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 respectively. 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	354	8% 50% 26% . 21%
1	B	354	3% 58% 24% . 16%
2	C	84	2% 52% 27% 20%
2	D	84	6% 46% 24% . 26%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5645 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	280	Total	C	N	O	S	0	0	0
			2229	1417	369	428	15			
1	B	296	Total	C	N	O	S	0	0	0
			2338	1483	386	453	16			

- Molecule 2 is a protein called GOLGI TO ER TRAFFIC PROTEIN 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	67	Total	C	N	O	0	0	0
			559	347	103	109			
2	D	62	Total	C	N	O	0	0	0
			518	322	93	103			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

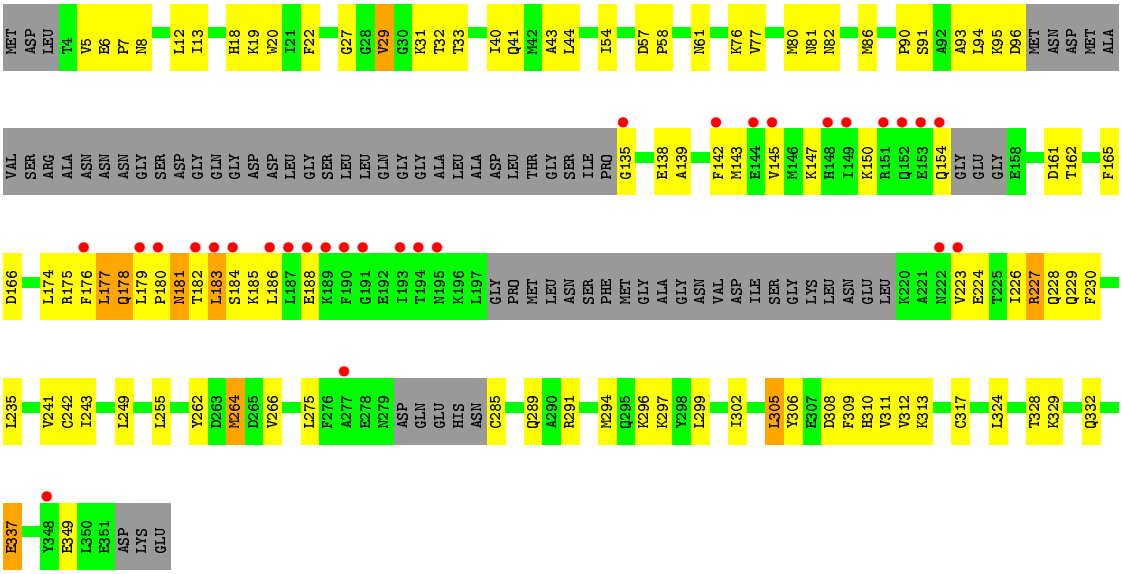
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

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 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 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.

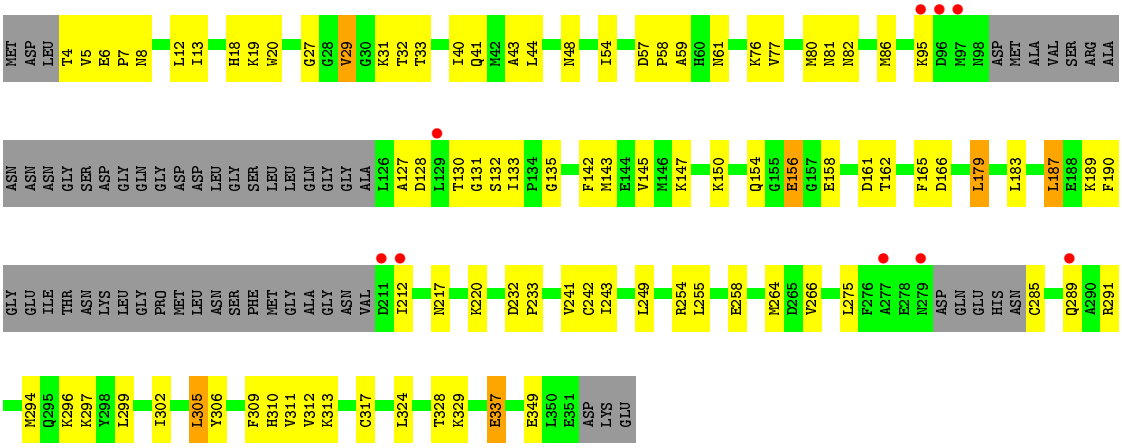
- Molecule 1: ATPASE GET3

Chain A:



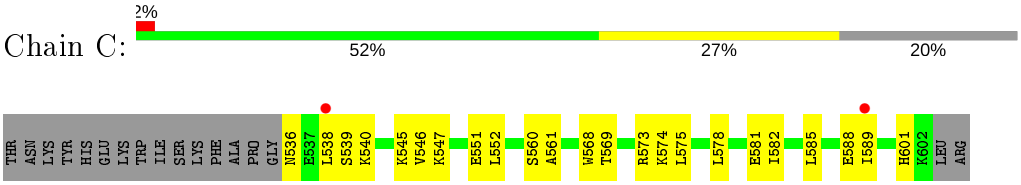
- Molecule 1: ATPASE GET3

Chain B:



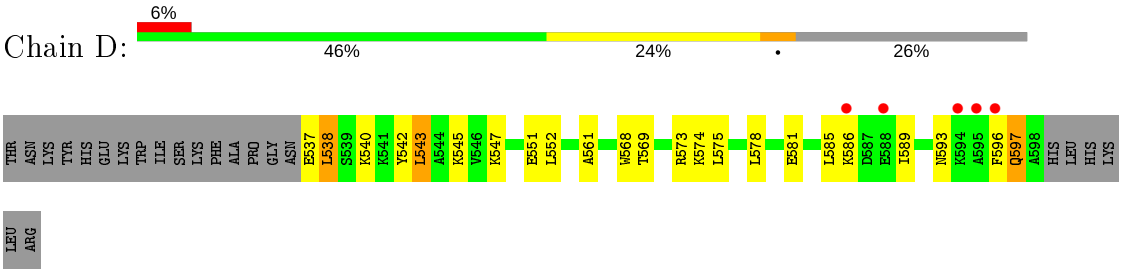
• Molecule 2: GOLGI TO ER TRAFFIC PROTEIN 1

Chain C:



• Molecule 2: GOLGI TO ER TRAFFIC PROTEIN 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	110.28Å 110.28Å 315.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.22 – 3.00 47.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.22-3.00) 98.9 (47.21-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.220 , 0.281 0.211 , 0.273	Depositor DCC
R_{free} test set	2339 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å^2)	86.7	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 68.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5645	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ZN

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	0.28	0/2265	0.48	0/3051
1	B	0.28	0/2376	0.46	0/3203
2	C	0.25	0/567	0.35	0/757
2	D	0.26	0/524	0.38	0/698
All	All	0.28	0/5732	0.45	0/7709

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	2229	0	2227	94	0
1	B	2338	0	2332	69	0
2	C	559	0	549	18	0
2	D	518	0	516	21	0
3	A	1	0	0	0	0
All	All	5645	0	5624	194	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 (194) 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:180:PRO:HB2	1:A:227:ARG:HB2	1.51	0.91
1:A:176:PHE:O	1:A:180:PRO:HD2	1.75	0.86
2:C:538:LEU:HD23	2:C:589:ILE:HD13	1.58	0.85
1:B:324:LEU:O	1:B:328:THR:HG23	1.79	0.83
1:A:324:LEU:O	1:A:328:THR:HG23	1.79	0.82
1:B:29:VAL:HG22	1:B:243:ILE:HG23	1.63	0.80
1:A:285:CYS:O	1:A:289:GLN:HG2	1.82	0.79
1:A:29:VAL:HG22	1:A:243:ILE:HG23	1.63	0.78
1:B:156:GLU:HG3	1:B:158:GLU:H	1.47	0.78
1:B:285:CYS:O	1:B:289:GLN:HG2	1.83	0.77
1:A:177:LEU:HD12	1:A:262:TYR:HB3	1.67	0.75
1:A:139:ALA:HB1	1:A:179:LEU:HD22	1.69	0.74
1:A:139:ALA:HB2	1:A:179:LEU:HD13	1.68	0.73
2:C:545:LYS:HE3	2:C:581:GLU:OE1	1.87	0.73
2:D:538:LEU:HD13	2:D:589:ILE:HD13	1.70	0.73
1:A:181:ASN:O	1:A:185:LYS:HG2	1.88	0.73
1:A:32:THR:HG21	1:A:61:ASN:HB3	1.71	0.72
1:B:128:ASP:HB3	2:C:546:VAL:HG11	1.71	0.72
1:B:32:THR:HG21	1:B:61:ASN:HB3	1.72	0.72
1:A:183:LEU:HD13	1:A:223:VAL:HG21	1.71	0.71
1:A:291:ARG:HD2	1:B:291:ARG:NH1	2.05	0.71
1:A:179:LEU:O	1:A:182:THR:N	2.24	0.69
1:B:306:TYR:HB3	1:B:309:PHE:CD1	2.27	0.69
1:A:179:LEU:O	1:A:183:LEU:N	2.17	0.69
1:A:95:LYS:O	1:A:95:LYS:HD3	1.93	0.69
1:A:29:VAL:HG21	1:A:242:CYS:HA	1.75	0.68
1:A:29:VAL:HG13	1:A:241:VAL:HG12	1.76	0.68
1:A:176:PHE:O	1:A:179:LEU:N	2.27	0.67
1:B:43:ALA:O	1:B:82:ASN:ND2	2.23	0.67
1:A:306:TYR:HB3	1:A:309:PHE:CD1	2.30	0.67
1:A:43:ALA:O	1:A:82:ASN:ND2	2.25	0.67
1:B:29:VAL:HG21	1:B:242:CYS:HA	1.76	0.67
1:B:29:VAL:HG13	1:B:241:VAL:HG12	1.76	0.66
1:B:76:LYS:HE3	1:B:81:ASN:O	1.94	0.66
2:D:542:TYR:HA	2:D:585:LEU:HD12	1.78	0.65
1:A:76:LYS:HE3	1:A:81:ASN:O	1.96	0.64
1:B:183:LEU:HD23	1:B:220:LYS:HB2	1.80	0.64
1:A:139:ALA:CB	1:A:179:LEU:HD22	2.28	0.64
2:D:538:LEU:HD22	2:D:589:ILE:HD11	1.78	0.64
2:D:545:LYS:HE3	2:D:581:GLU:OE2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:CG2	1:A:243:ILE:HG23	2.29	0.63
1:A:176:PHE:O	1:A:180:PRO:CD	2.48	0.62
1:A:291:ARG:NH1	1:B:291:ARG:HD2	2.14	0.62
1:B:4:THR:HG22	1:B:5:VAL:H	1.65	0.62
2:D:542:TYR:CE2	2:D:586:LYS:HG3	2.35	0.61
1:B:29:VAL:CG2	1:B:243:ILE:HG23	2.28	0.61
2:D:542:TYR:HE2	2:D:586:LYS:HG3	1.65	0.61
1:A:6:GLU:HB3	1:A:8:ASN:HD21	1.65	0.60
1:A:174:LEU:O	1:A:177:LEU:N	2.35	0.59
1:B:6:GLU:HB3	1:B:8:ASN:HD21	1.67	0.59
1:B:305:LEU:HD22	2:D:573:ARG:HH22	1.67	0.59
2:D:552:LEU:HB3	2:D:575:LEU:HD21	1.85	0.59
1:A:18:HIS:O	1:A:162:THR:OG1	2.19	0.58
1:A:6:GLU:HB3	1:A:8:ASN:ND2	2.18	0.58
1:B:305:LEU:HD11	2:D:569:THR:HG21	1.85	0.58
2:C:552:LEU:HB3	2:C:575:LEU:HD21	1.85	0.58
1:A:329:LYS:NZ	1:A:349:GLU:OE1	2.37	0.58
1:B:142:PHE:O	1:B:145:VAL:HG22	2.03	0.58
1:A:142:PHE:O	1:A:145:VAL:HG22	2.04	0.58
1:B:329:LYS:NZ	1:B:349:GLU:OE1	2.37	0.57
1:A:174:LEU:HD22	1:A:177:LEU:HB2	1.86	0.57
1:A:179:LEU:HA	1:A:182:THR:OG1	2.05	0.57
1:B:6:GLU:HB3	1:B:8:ASN:ND2	2.20	0.56
1:A:177:LEU:HD22	1:A:230:PHE:CD2	2.40	0.56
1:A:178:GLN:O	1:A:182:THR:HG23	2.05	0.56
1:A:13:ILE:HD13	1:A:41:GLN:HB3	1.88	0.55
1:A:179:LEU:HG	1:A:183:LEU:HB2	1.89	0.55
1:B:179:LEU:O	1:B:183:LEU:N	2.38	0.54
1:B:13:ILE:HD13	1:B:41:GLN:HB3	1.88	0.54
1:A:184:SER:O	1:A:188:GLU:HG3	2.08	0.54
1:A:93:ALA:O	1:A:96:ASP:HB2	2.08	0.54
1:A:179:LEU:HD12	1:A:182:THR:OG1	2.07	0.54
1:A:305:LEU:HD11	2:C:569:THR:HG21	1.90	0.53
2:D:597:GLN:N	2:D:597:GLN:OE1	2.42	0.53
1:A:22:PHE:CD2	1:A:264:MET:HE1	2.43	0.53
1:B:150:LYS:HE3	1:B:154:GLN:HG2	1.91	0.53
1:A:90:PRO:O	1:A:94:LEU:HB2	2.09	0.53
1:A:223:VAL:O	1:A:226:ILE:HB	2.10	0.52
1:B:127:ALA:HA	1:B:130:THR:HG22	1.90	0.52
1:B:156:GLU:HG3	1:B:158:GLU:N	2.21	0.52
1:A:150:LYS:HE3	1:A:154:GLN:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:HIS:O	1:B:162:THR:OG1	2.24	0.52
1:A:305:LEU:HD22	2:C:573:ARG:HH22	1.74	0.52
1:A:275:LEU:HD11	1:A:291:ARG:HD3	1.92	0.51
1:B:130:THR:HG23	1:B:131:GLY:H	1.75	0.51
1:B:7:PRO:HG2	1:B:337:GLU:HG2	1.92	0.51
2:C:536:ASN:O	2:C:540:LYS:HG3	2.11	0.51
1:B:275:LEU:HD11	1:B:291:ARG:HD3	1.92	0.51
2:C:538:LEU:HD21	2:C:588:GLU:HB3	1.93	0.51
1:B:296:LYS:HA	1:B:299:LEU:HB2	1.92	0.51
1:A:95:LYS:C	1:A:95:LYS:HD3	2.30	0.50
2:C:538:LEU:HD21	2:C:588:GLU:CB	2.41	0.50
1:A:185:LYS:HD3	1:A:185:LYS:N	2.27	0.50
1:B:130:THR:HG23	1:B:131:GLY:N	2.27	0.50
1:A:296:LYS:HA	1:A:299:LEU:HB2	1.94	0.50
1:A:80:MET:HG2	1:A:324:LEU:HD21	1.93	0.49
1:B:95:LYS:O	1:B:95:LYS:HD3	2.12	0.49
1:A:139:ALA:CB	1:A:179:LEU:HD13	2.39	0.49
2:C:585:LEU:O	2:C:589:ILE:HG12	2.13	0.49
2:D:561:ALA:HB2	2:D:568:TRP:CE2	2.48	0.48
2:C:561:ALA:HB2	2:C:568:TRP:CE2	2.48	0.48
1:A:143:MET:O	1:A:147:LYS:HG3	2.14	0.48
1:A:177:LEU:O	1:A:177:LEU:HD13	2.13	0.48
1:A:299:LEU:HD22	1:A:313:LYS:HE3	1.94	0.48
1:B:183:LEU:HD23	1:B:220:LYS:CB	2.44	0.48
1:A:229:GLN:HA	1:A:235:LEU:HD12	1.94	0.48
1:B:80:MET:HG2	1:B:324:LEU:HD21	1.95	0.48
1:A:177:LEU:HD22	1:A:230:PHE:HD2	1.77	0.48
1:A:249:LEU:HD21	1:A:302:ILE:HD11	1.96	0.48
1:B:20:TRP:HE3	1:B:165:PHE:HE2	1.60	0.48
1:A:20:TRP:HE3	1:A:165:PHE:HE2	1.62	0.47
1:A:57:ASP:OD1	1:A:58:PRO:HD2	2.15	0.47
1:B:57:ASP:OD1	1:B:58:PRO:HD2	2.14	0.47
1:A:7:PRO:HG2	1:A:337:GLU:HG2	1.96	0.47
1:A:294:MET:O	1:A:297:LYS:HB3	2.15	0.47
1:A:176:PHE:CD1	1:A:179:LEU:HB3	2.50	0.46
2:C:536:ASN:HB3	2:C:539:SER:HB3	1.98	0.46
1:B:132:SER:OG	1:B:133:ILE:HD12	2.15	0.46
2:C:552:LEU:HD23	2:C:575:LEU:HD23	1.98	0.46
2:D:538:LEU:HD22	2:D:589:ILE:CD1	2.44	0.46
1:B:133:ILE:N	1:B:133:ILE:HD12	2.31	0.46
1:B:299:LEU:HD22	1:B:313:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:552:LEU:HD23	2:D:575:LEU:HD23	1.98	0.46
1:A:54:ILE:HG13	1:A:86:MET:HB2	1.98	0.45
1:B:5:VAL:HG13	1:B:310:HIS:CE1	2.52	0.45
1:A:229:GLN:HG2	1:A:235:LEU:HD13	1.98	0.45
1:B:179:LEU:HD13	1:B:183:LEU:HB2	1.98	0.45
1:B:294:MET:O	1:B:297:LYS:HB3	2.17	0.45
1:B:27:GLY:C	1:B:29:VAL:H	2.19	0.45
1:B:31:LYS:HE3	1:B:166:ASP:OD1	2.16	0.45
1:B:249:LEU:HD21	1:B:302:ILE:HD11	1.97	0.45
1:B:4:THR:HG22	1:B:5:VAL:N	2.31	0.45
2:D:537:GLU:N	2:D:540:LYS:HZ3	2.15	0.45
2:D:542:TYR:CD1	2:D:543:LEU:N	2.85	0.45
1:B:135:GLY:HA3	1:B:179:LEU:HD23	1.98	0.45
1:B:150:LYS:HD2	1:B:150:LYS:HA	1.78	0.45
1:B:187:LEU:HA	1:B:187:LEU:HD22	1.85	0.44
1:A:29:VAL:CG2	1:A:242:CYS:HA	2.44	0.44
1:B:143:MET:O	1:B:147:LYS:HG3	2.16	0.44
2:D:585:LEU:O	2:D:589:ILE:HG12	2.17	0.44
1:A:138:GLU:HB2	1:A:175:ARG:HB3	1.99	0.44
1:B:54:ILE:HG13	1:B:86:MET:HB2	1.98	0.44
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.75	0.44
1:B:305:LEU:HD13	1:B:306:TYR:CZ	2.52	0.44
1:A:142:PHE:CD1	1:A:176:PHE:CD2	3.06	0.44
1:A:5:VAL:HG13	1:A:310:HIS:CE1	2.53	0.44
1:A:27:GLY:C	1:A:29:VAL:H	2.21	0.43
1:A:31:LYS:HB3	1:A:31:LYS:HE2	1.75	0.43
1:A:183:LEU:O	1:A:186:LEU:HB3	2.18	0.43
1:A:227:ARG:NH1	1:A:228:GLN:HG2	2.33	0.43
1:B:232:ASP:HA	1:B:233:PRO:HD2	1.90	0.43
2:C:536:ASN:CB	2:C:539:SER:HB3	2.49	0.43
2:C:547:LYS:HE2	2:C:551:GLU:OE2	2.18	0.43
1:A:135:GLY:HA2	1:A:175:ARG:HG3	2.01	0.43
1:A:43:ALA:HB1	1:A:82:ASN:OD1	2.19	0.42
1:A:305:LEU:HD13	1:A:306:TYR:CZ	2.54	0.42
1:B:31:LYS:HE2	1:B:31:LYS:HB3	1.76	0.42
1:A:176:PHE:C	1:A:179:LEU:H	2.21	0.42
1:A:181:ASN:O	1:A:185:LYS:HE2	2.19	0.42
1:A:40:ILE:O	1:A:44:LEU:HG	2.19	0.42
1:B:29:VAL:O	1:B:29:VAL:HG13	2.20	0.42
1:B:43:ALA:HB1	1:B:82:ASN:OD1	2.20	0.42
1:B:59:ALA:HB2	2:C:560:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PHE:CD1	1:A:176:PHE:CE2	3.08	0.42
1:B:40:ILE:O	1:B:44:LEU:HG	2.20	0.42
1:A:20:TRP:CE3	1:A:165:PHE:HE2	2.38	0.42
1:A:179:LEU:HD12	1:A:182:THR:HG1	1.84	0.42
1:A:80:MET:HE3	1:A:80:MET:HB3	1.95	0.42
1:B:266:VAL:O	1:B:266:VAL:HG13	2.20	0.42
2:C:574:LYS:HE3	2:C:578:LEU:HD21	2.01	0.42
2:D:542:TYR:CD1	2:D:542:TYR:C	2.93	0.41
1:A:19:LYS:HG3	1:A:161:ASP:O	2.20	0.41
1:B:29:VAL:CG2	1:B:242:CYS:HA	2.45	0.41
1:A:266:VAL:O	1:A:266:VAL:HG13	2.21	0.41
1:A:138:GLU:CG	1:A:175:ARG:HB3	2.51	0.41
1:B:48:ASN:N	1:B:48:ASN:OD1	2.48	0.41
2:D:547:LYS:HE2	2:D:551:GLU:OE2	2.20	0.41
1:A:150:LYS:HA	1:A:150:LYS:HD2	1.77	0.41
1:B:20:TRP:CE3	1:B:165:PHE:HE2	2.37	0.41
1:B:189:LYS:HD3	1:B:189:LYS:HA	1.91	0.41
1:B:190:PHE:CD1	1:B:190:PHE:C	2.93	0.41
1:B:254:ARG:NH2	1:B:258:GLU:OE1	2.53	0.41
1:A:135:GLY:HA2	1:A:175:ARG:CG	2.51	0.41
1:A:91:SER:O	1:A:94:LEU:HB3	2.21	0.41
2:D:574:LYS:HE3	2:D:578:LEU:HD21	2.03	0.41
1:A:31:LYS:HE3	1:A:166:ASP:OD1	2.21	0.40
1:A:308:ASP:N	1:A:308:ASP:OD1	2.47	0.40
2:C:552:LEU:HD23	2:C:575:LEU:CD2	2.52	0.40
1:A:138:GLU:CB	1:A:175:ARG:HB3	2.51	0.40
1:A:329:LYS:O	1:A:332:GLN:HG2	2.21	0.40
1:B:19:LYS:HG3	1:B:161:ASP:O	2.22	0.40
2:D:552:LEU:HD23	2:D:575:LEU:CD2	2.51	0.40
2:D:593:ASN:O	2:D:596:PHE:HB3	2.21	0.40
1:B:80:MET:HB3	1:B:80:MET:HE3	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	270/354 (76%)	267 (99%)	3 (1%)	0	100	100
1	B	288/354 (81%)	285 (99%)	3 (1%)	0	100	100
2	C	65/84 (77%)	64 (98%)	1 (2%)	0	100	100
2	D	60/84 (71%)	58 (97%)	2 (3%)	0	100	100
All	All	683/876 (78%)	674 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/309 (82%)	236 (93%)	17 (7%)	16	49
1	B	265/309 (86%)	249 (94%)	16 (6%)	19	53
2	C	61/77 (79%)	59 (97%)	2 (3%)	38	73
2	D	57/77 (74%)	54 (95%)	3 (5%)	22	58
All	All	636/772 (82%)	598 (94%)	38 (6%)	19	53

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	29	VAL
1	A	33	THR
1	A	77	VAL
1	A	177	LEU
1	A	178	GLN
1	A	181	ASN
1	A	183	LEU
1	A	224	GLU
1	A	227	ARG

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Mol	Chain	Res	Type
1	A	255	LEU
1	A	264	MET
1	A	305	LEU
1	A	311	VAL
1	A	312	VAL
1	A	317	CYS
1	A	337	GLU
1	B	12	LEU
1	B	29	VAL
1	B	33	THR
1	B	77	VAL
1	B	156	GLU
1	B	179	LEU
1	B	187	LEU
1	B	212	ILE
1	B	217	ASN
1	B	255	LEU
1	B	264	MET
1	B	305	LEU
1	B	311	VAL
1	B	312	VAL
1	B	317	CYS
1	B	337	GLU
2	C	582	ILE
2	C	601	HIS
2	D	538	LEU
2	D	543	LEU
2	D	597	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 1 ligands modelled in this entry, 1 is 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, 95^{th} 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	280/354 (79%)	0.38	29 (10%) 6 2	61, 98, 198, 343	0
1	B	296/354 (83%)	0.09	9 (3%) 50 22	58, 96, 170, 211	0
2	C	67/84 (79%)	0.03	2 (2%) 50 22	80, 112, 150, 182	0
2	D	62/84 (73%)	0.29	5 (8%) 12 3	70, 111, 178, 205	0
All	All	705/876 (80%)	0.22	45 (6%) 19 6	58, 101, 179, 343	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	PHE	7.9
1	A	148	HIS	5.5
1	A	191	GLY	5.2
1	A	195	ASN	4.8
1	A	135	GLY	4.8
1	A	187	LEU	4.7
1	A	151	ARG	4.7
1	A	186	LEU	4.6
1	A	277	ALA	4.6
1	A	145	VAL	4.4
1	A	176	PHE	4.4
2	D	594	LYS	4.1
1	B	96	ASP	3.7
1	A	193	ILE	3.6
1	A	149	ILE	3.2
1	B	95	LYS	3.2
1	B	277	ALA	3.2
1	B	211	ASP	3.2
1	B	129	LEU	3.1
1	A	179	LEU	3.0
1	A	153	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	180	PRO	2.9
1	A	152	GLN	2.7
1	A	184	SER	2.7
1	B	212	ILE	2.7
1	A	142	PHE	2.6
1	A	194	THR	2.6
1	A	183	LEU	2.6
1	A	348	TYR	2.5
1	A	189	LYS	2.4
1	B	289	GLN	2.4
1	A	223	VAL	2.4
2	C	538	LEU	2.4
1	A	182	THR	2.3
1	B	97	MET	2.3
2	D	596	PHE	2.3
1	A	144	GLU	2.2
1	A	188	GLU	2.2
2	D	588	GLU	2.2
1	A	154	GLN	2.1
2	D	586	LYS	2.1
1	B	279	ASN	2.0
2	C	589	ILE	2.0
2	D	595	ALA	2.0
1	A	222	ASN	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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
3	ZN	A	1352	1/1	0.98	0.09	114,114,114,114	0

6.5 Other polymers (i)

There are no such residues in this entry.