



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2021 – 02:06 PM EDT

PDB ID : 7JQP
Title : The Phi-28 gp11 DNA packaging Motor
Authors : Morais, M.C.; White, M.A.; Dill, E.
Deposited on : 2020-08-11
Resolution : 2.89 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
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)	:	2.20

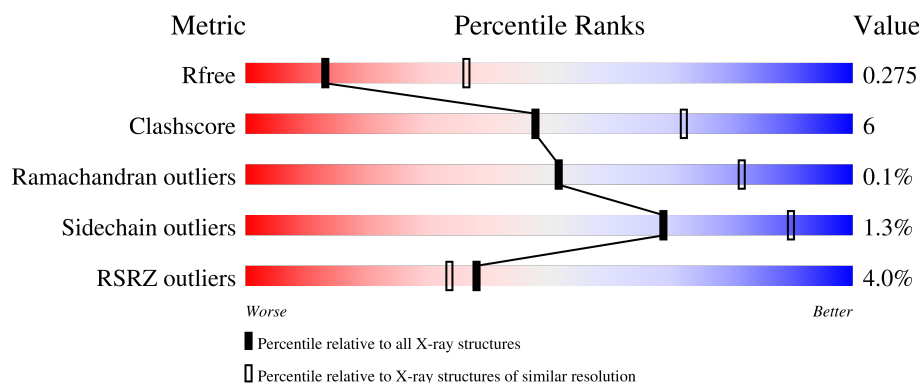
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of 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 $\leq 5\%$. 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	374	<div> <div>3%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	B	374	<div> <div>2%</div> <div>81%</div> <div>15%</div> <div>.</div> </div>
1	C	374	<div> <div>4%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	D	374	<div> <div>5%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
1	E	374	<div> <div>4%</div> <div>81%</div> <div>15%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29716 atoms, of which 14620 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 Encapsidation protein.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	364	Total	C	H	N	O	S	Se		0	0	0
			5938	1959	2915	493	561	2	8				
1	B	360	Total	C	H	N	O	S	Se		0	0	0
			5876	1939	2888	489	550	2	8				
1	C	362	Total	C	H	N	O	S	Se		0	0	0
			5944	1957	2926	493	558	2	8				
1	D	361	Total	C	H	N	O	S	Se		0	0	0
			5954	1957	2940	492	555	2	8				
1	E	361	Total	C	H	N	O	S	Se		0	0	0
			5973	1960	2951	497	555	2	8				

There are 40 discrepancies between the modelled and reference sequences:

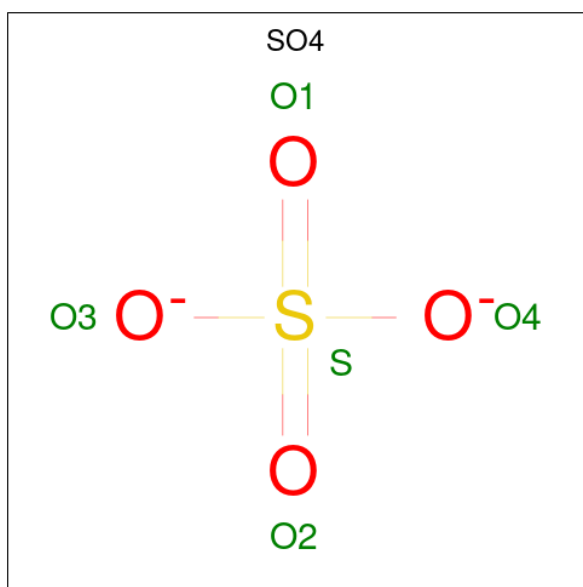
Chain	Residue	Modelled	Actual	Comment	Reference
A	367	LEU	-	expression tag	UNP B1ABI1
A	368	GLU	-	expression tag	UNP B1ABI1
A	369	HIS	-	expression tag	UNP B1ABI1
A	370	HIS	-	expression tag	UNP B1ABI1
A	371	HIS	-	expression tag	UNP B1ABI1
A	372	HIS	-	expression tag	UNP B1ABI1
A	373	HIS	-	expression tag	UNP B1ABI1
A	374	HIS	-	expression tag	UNP B1ABI1
B	367	LEU	-	expression tag	UNP B1ABI1
B	368	GLU	-	expression tag	UNP B1ABI1
B	369	HIS	-	expression tag	UNP B1ABI1
B	370	HIS	-	expression tag	UNP B1ABI1
B	371	HIS	-	expression tag	UNP B1ABI1
B	372	HIS	-	expression tag	UNP B1ABI1
B	373	HIS	-	expression tag	UNP B1ABI1
B	374	HIS	-	expression tag	UNP B1ABI1
C	367	LEU	-	expression tag	UNP B1ABI1
C	368	GLU	-	expression tag	UNP B1ABI1
C	369	HIS	-	expression tag	UNP B1ABI1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	370	HIS	-	expression tag	UNP B1ABI1
C	371	HIS	-	expression tag	UNP B1ABI1
C	372	HIS	-	expression tag	UNP B1ABI1
C	373	HIS	-	expression tag	UNP B1ABI1
C	374	HIS	-	expression tag	UNP B1ABI1
D	367	LEU	-	expression tag	UNP B1ABI1
D	368	GLU	-	expression tag	UNP B1ABI1
D	369	HIS	-	expression tag	UNP B1ABI1
D	370	HIS	-	expression tag	UNP B1ABI1
D	371	HIS	-	expression tag	UNP B1ABI1
D	372	HIS	-	expression tag	UNP B1ABI1
D	373	HIS	-	expression tag	UNP B1ABI1
D	374	HIS	-	expression tag	UNP B1ABI1
E	367	LEU	-	expression tag	UNP B1ABI1
E	368	GLU	-	expression tag	UNP B1ABI1
E	369	HIS	-	expression tag	UNP B1ABI1
E	370	HIS	-	expression tag	UNP B1ABI1
E	371	HIS	-	expression tag	UNP B1ABI1
E	372	HIS	-	expression tag	UNP B1ABI1
E	373	HIS	-	expression tag	UNP B1ABI1
E	374	HIS	-	expression tag	UNP B1ABI1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

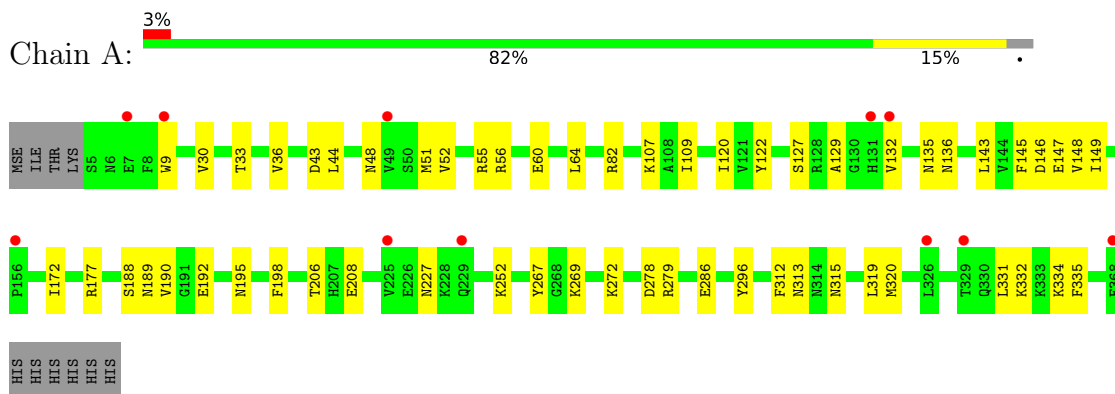
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	3	Total	O	0	0
			3	3		
3	D	2	Total	O	0	0
			2	2		

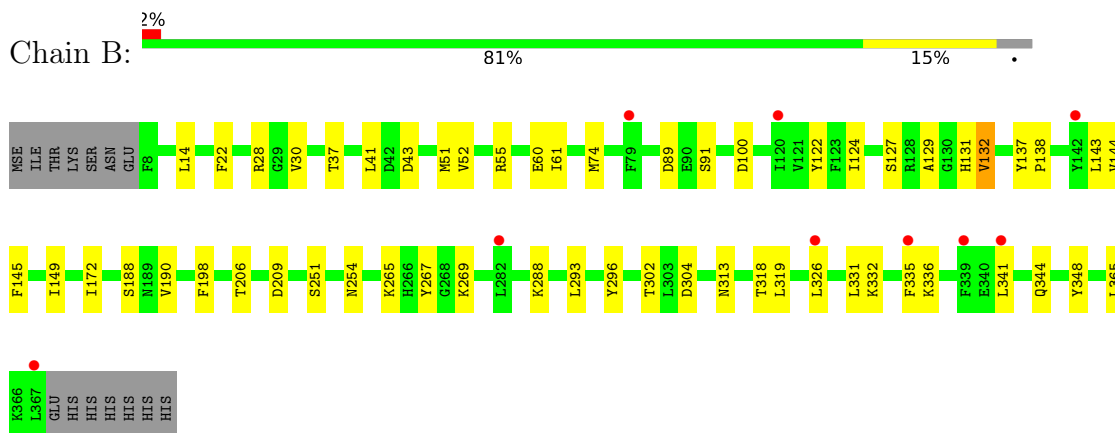
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

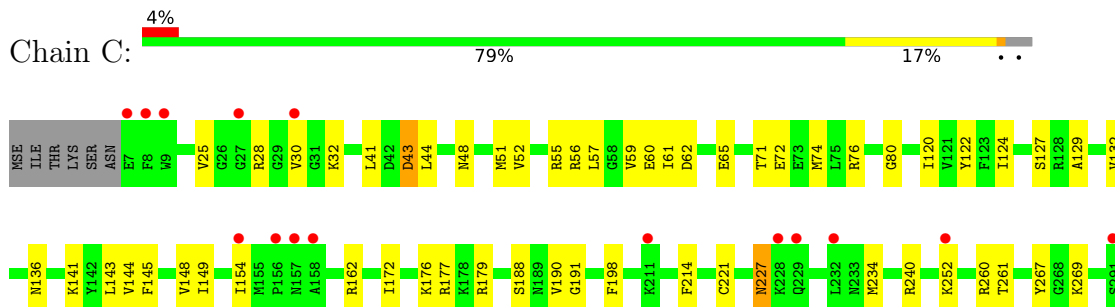
• Molecule 1: Encapsidation protein

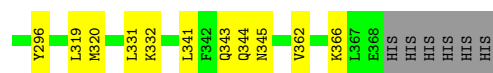


• Molecule 1: Encapsidation protein

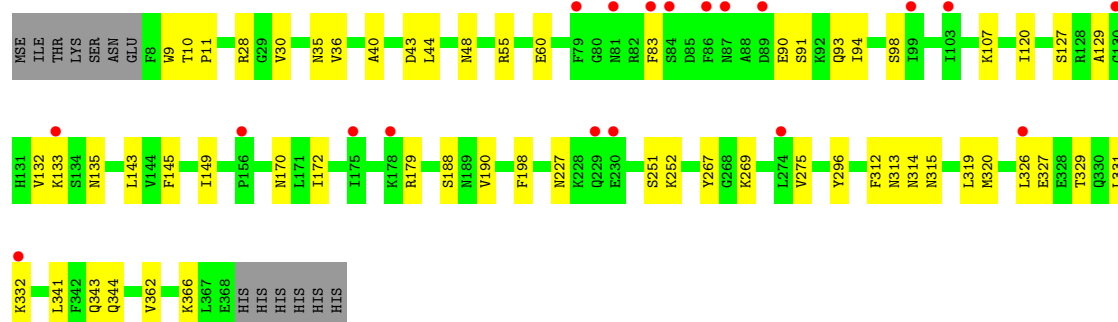
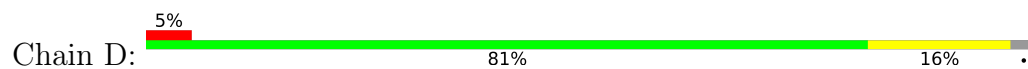


• Molecule 1: Encapsidation protein

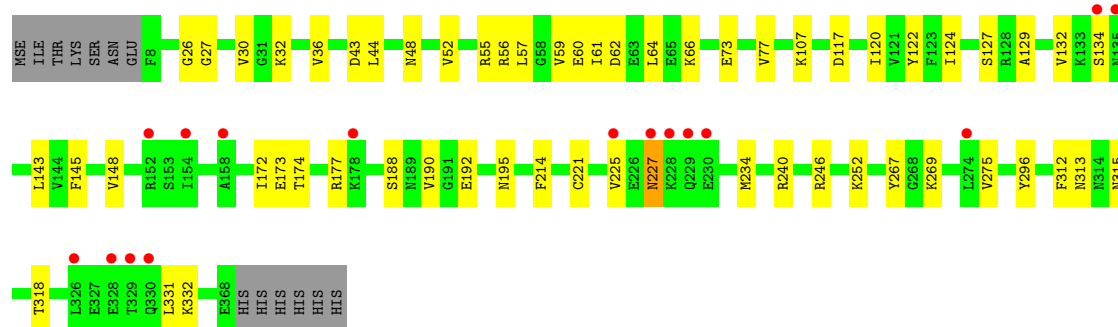
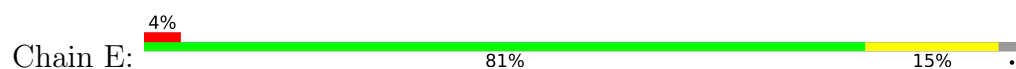




• Molecule 1: Encapsidation protein



• Molecule 1: Encapsidation protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.90Å 110.90Å 351.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.13 – 2.89 50.13 – 2.89	Depositor EDS
% Data completeness (in resolution range)	77.4 (50.13-2.89) 71.5 (50.13-2.89)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.226 , 0.276 0.226 , 0.275	Depositor DCC
R_{free} test set	2000 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	29716	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: SO4

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	0/3086	0.47	0/4153
1	B	0.28	0/3051	0.50	0/4107
1	C	0.28	0/3081	0.47	0/4144
1	D	0.29	0/3077	0.48	0/4136
1	E	0.27	0/3085	0.47	0/4146
All	All	0.28	0/15380	0.48	0/20686

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	3023	2915	2915	35	0
1	B	2988	2888	2888	35	0
1	C	3018	2926	2926	44	0
1	D	3014	2940	2940	40	0
1	E	3022	2951	2951	37	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	5	0	0	0	0
2	E	5	0	0	0	0
3	A	1	0	0	1	0
3	B	3	0	0	1	0
3	D	2	0	0	1	0
All	All	15096	14620	14620	182	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 6.

All (182) 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:147:GLU:OE2	1:A:189:ASN:ND2	1.94	1.01
1:E:227:ASN:ND2	1:E:252:LYS:O	2.03	0.91
1:B:55:ARG:NH1	1:B:60:GLU:OE1	2.08	0.87
1:E:55:ARG:NH1	1:E:60:GLU:OE1	2.10	0.85
1:D:55:ARG:NH1	1:D:60:GLU:OE1	2.12	0.82
1:B:331:LEU:HD21	1:B:365:LEU:HD23	1.60	0.82
1:C:176:LYS:NZ	1:C:179:ARG:O	2.12	0.82
1:C:55:ARG:NH1	1:C:60:GLU:OE1	2.15	0.80
1:D:227:ASN:ND2	1:D:252:LYS:O	2.16	0.79
1:A:227:ASN:ND2	1:A:252:LYS:O	2.16	0.78
1:C:188:SER:OG	1:C:190:VAL:O	2.02	0.77
1:B:28:ARG:NH1	1:B:251:SER:O	2.17	0.77
1:A:82:ARG:O	3:A:601:HOH:O	2.06	0.74
1:A:55:ARG:NH1	1:A:60:GLU:OE1	2.21	0.73
1:A:149:ILE:HD11	1:A:198:PHE:CE1	2.24	0.73
1:D:343:GLN:HG3	1:D:366:LYS:NZ	2.03	0.72
1:D:90:GLU:O	1:D:91:SER:OG	2.08	0.72
1:A:312:PHE:CZ	1:A:334:LYS:NZ	2.58	0.71
1:B:313:ASN:HD21	1:B:318:THR:HG23	1.55	0.71
1:E:107:LYS:NZ	1:E:117:ASP:OD1	2.17	0.70
1:B:188:SER:OG	1:B:190:VAL:O	2.09	0.70
1:E:188:SER:OG	1:E:190:VAL:O	2.10	0.69
1:B:28:ARG:NH2	1:B:254:ASN:OD1	2.27	0.67
1:A:206:THR:OG1	1:A:208:GLU:OE1	2.12	0.67
1:A:188:SER:OG	1:A:190:VAL:O	2.13	0.66
1:C:56:ARG:NH2	1:C:148:VAL:O	2.27	0.64
1:B:100:ASP:N	3:B:601:HOH:O	2.32	0.62
1:D:331:LEU:HD12	1:D:332:LYS:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:SER:OG	1:D:190:VAL:O	2.17	0.61
1:B:51:MSE:HE3	1:B:144:VAL:HG21	1.83	0.60
1:B:132:VAL:HG23	1:B:132:VAL:O	2.01	0.60
1:D:343:GLN:HG3	1:D:366:LYS:HZ1	1.67	0.60
1:D:149:ILE:HD11	1:D:198:PHE:CE1	2.37	0.59
1:B:302:THR:HG21	1:B:304:ASP:OD2	2.02	0.59
1:C:149:ILE:HD11	1:C:198:PHE:CE1	2.38	0.58
1:A:331:LEU:HD12	1:A:332:LYS:N	2.18	0.58
1:D:94:ILE:HD11	1:D:107:LYS:HE2	1.86	0.58
1:B:52:VAL:HG22	1:B:122:TYR:HB2	1.86	0.57
1:A:30:VAL:O	1:A:30:VAL:HG12	2.05	0.56
1:E:234:MSE:O	1:E:240:ARG:NH1	2.31	0.56
1:E:30:VAL:O	1:E:30:VAL:HG12	2.06	0.56
1:A:136:ASN:OD1	1:A:177:ARG:NH1	2.38	0.56
1:D:30:VAL:HG12	1:D:30:VAL:O	2.06	0.55
1:E:331:LEU:HD12	1:E:332:LYS:N	2.22	0.55
1:B:149:ILE:HD11	1:B:198:PHE:CE1	2.42	0.55
1:C:331:LEU:HD12	1:C:332:LYS:N	2.22	0.54
1:B:302:THR:CG2	1:B:304:ASP:OD2	2.56	0.54
1:E:129:ALA:O	1:E:132:VAL:HG22	2.08	0.54
1:E:143:LEU:HD23	1:E:172:ILE:HD13	1.89	0.54
1:E:56:ARG:NH2	1:E:148:VAL:O	2.31	0.53
1:C:267:TYR:HB2	1:C:296:TYR:CD2	2.44	0.53
1:D:252:LYS:CE	1:E:173:GLU:OE1	2.56	0.53
1:D:143:LEU:HD23	1:D:172:ILE:HD13	1.91	0.53
1:C:267:TYR:CZ	1:C:269:LYS:HB2	2.43	0.53
1:D:267:TYR:CE2	1:D:269:LYS:HB2	2.43	0.53
1:B:331:LEU:HD21	1:B:365:LEU:CD2	2.35	0.53
1:D:83:PHE:HA	1:D:98:SER:O	2.08	0.53
1:B:30:VAL:HG12	1:B:30:VAL:O	2.09	0.52
1:C:72:GLU:OE2	1:C:76:ARG:NH2	2.40	0.52
1:E:313:ASN:OD1	1:E:318:THR:HG23	2.09	0.52
1:C:30:VAL:HG12	1:C:30:VAL:O	2.09	0.51
1:D:93:GLN:O	1:D:107:LYS:HA	2.11	0.51
1:A:267:TYR:CE2	1:A:269:LYS:HB2	2.45	0.51
1:D:319:LEU:HD23	1:D:320:MSE:N	2.26	0.51
1:E:315:ASN:HB3	1:E:318:THR:HG22	1.92	0.51
1:B:332:LYS:O	1:B:336:LYS:HB2	2.12	0.50
1:D:28:ARG:NH2	1:D:251:SER:OG	2.33	0.50
1:A:278:ASP:OD1	1:E:246:ARG:NH2	2.45	0.50
1:C:319:LEU:HD23	1:C:320:MSE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:VAL:O	1:D:366:LYS:HB2	2.11	0.49
1:B:14:LEU:HD23	1:B:22:PHE:CD1	2.47	0.49
1:B:331:LEU:CD2	1:B:365:LEU:HD23	2.39	0.49
1:E:313:ASN:OD1	1:E:315:ASN:O	2.30	0.49
1:A:192:GLU:O	1:A:195:ASN:ND2	2.45	0.49
1:A:319:LEU:HD23	1:A:320:MSE:N	2.28	0.49
1:C:267:TYR:CE2	1:C:269:LYS:HB2	2.48	0.49
1:C:32:LYS:N	2:C:500:SO4:O4	2.46	0.49
1:C:162:ARG:NE	1:C:366:LYS:O	2.46	0.49
1:D:179:ARG:NH1	3:D:601:HOH:O	2.38	0.49
1:D:327:GLU:OE2	1:D:329:THR:OG1	2.22	0.49
1:C:136:ASN:OD1	1:C:177:ARG:NH1	2.47	0.48
1:B:129:ALA:O	1:B:132:VAL:HG22	2.13	0.48
1:E:267:TYR:CE2	1:E:269:LYS:HB2	2.48	0.48
1:A:52:VAL:HG22	1:A:122:TYR:HB2	1.95	0.48
1:B:267:TYR:CE2	1:B:269:LYS:HB2	2.48	0.48
1:C:234:MSE:O	1:C:240:ARG:NH1	2.39	0.48
1:E:59:VAL:HA	1:E:62:ASP:HB2	1.95	0.48
1:D:267:TYR:HB2	1:D:296:TYR:CD2	2.49	0.48
1:D:252:LYS:HE3	1:E:173:GLU:OE1	2.14	0.47
1:D:343:GLN:CG	1:D:366:LYS:NZ	2.75	0.47
1:E:192:GLU:O	1:E:195:ASN:ND2	2.47	0.47
1:A:129:ALA:O	1:A:132:VAL:HG22	2.14	0.47
1:B:143:LEU:HD23	1:B:172:ILE:HD13	1.97	0.47
1:B:319:LEU:C	1:B:319:LEU:HD23	2.35	0.47
1:C:143:LEU:HD23	1:C:172:ILE:HD13	1.97	0.47
1:C:43:ASP:OD2	1:C:141:LYS:NZ	2.44	0.47
1:A:272:LYS:NZ	1:A:286:GLU:OE1	2.36	0.47
1:E:313:ASN:OD1	1:E:318:THR:CG2	2.63	0.46
1:A:334:LYS:HG3	1:A:335:PHE:N	2.30	0.46
1:C:227:ASN:ND2	1:C:252:LYS:O	2.48	0.46
1:A:312:PHE:CE1	1:A:334:LYS:NZ	2.83	0.46
1:A:33:THR:OG1	1:A:146:ASP:OD2	2.26	0.46
1:C:341:LEU:O	1:C:344:GLN:O	2.34	0.46
1:E:44:LEU:HD23	1:E:120:ILE:HB	1.96	0.46
1:E:73:GLU:O	1:E:77:VAL:HG23	2.15	0.46
1:E:134:SER:O	1:E:177:ARG:NH1	2.48	0.46
1:A:143:LEU:HD23	1:A:172:ILE:HD13	1.98	0.45
1:B:61:ILE:HD11	1:B:124:ILE:O	2.16	0.45
1:D:11:PRO:HG3	1:D:36:VAL:HA	1.98	0.45
1:E:32:LYS:O	1:E:36:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:VAL:HG22	1:E:122:TYR:HB2	1.98	0.45
1:C:176:LYS:CE	1:C:179:ARG:O	2.64	0.45
1:A:267:TYR:HB2	1:A:296:TYR:CD2	2.51	0.45
1:A:279:ARG:HG3	1:E:246:ARG:HH12	1.82	0.45
1:D:129:ALA:O	1:D:132:VAL:HG22	2.17	0.45
1:C:51:MSE:HE2	1:C:144:VAL:CG2	2.47	0.44
1:C:362:VAL:O	1:C:366:LYS:HB2	2.17	0.44
1:C:41:LEU:HD21	1:C:74:MSE:CE	2.47	0.44
1:C:129:ALA:O	1:C:132:VAL:HG22	2.17	0.44
1:E:267:TYR:HB2	1:E:296:TYR:CD2	2.53	0.44
1:B:41:LEU:HD21	1:B:74:MSE:CE	2.47	0.44
1:C:76:ARG:O	1:C:80:GLY:N	2.48	0.44
1:A:208:GLU:OE1	1:A:208:GLU:N	2.39	0.44
1:A:56:ARG:NH2	1:A:148:VAL:O	2.37	0.44
1:A:51:MSE:HG2	1:A:52:VAL:N	2.33	0.44
1:C:52:VAL:HG22	1:C:122:TYR:HB2	2.00	0.44
1:D:314:ASN:HA	1:D:326:LEU:HB3	2.00	0.44
1:B:288:LYS:HD3	1:B:293:LEU:HD11	1.99	0.44
1:C:331:LEU:HD12	1:C:331:LEU:C	2.38	0.44
1:B:89:ASP:OD1	1:B:91:SER:OG	2.33	0.43
1:E:61:ILE:HD11	1:E:124:ILE:O	2.18	0.43
1:B:267:TYR:HB2	1:B:296:TYR:CD2	2.53	0.43
1:B:137:TYR:N	1:B:138:PRO:HD3	2.34	0.43
1:C:44:LEU:HD23	1:C:120:ILE:HB	1.99	0.43
1:C:59:VAL:HA	1:C:62:ASP:HB2	1.99	0.43
1:C:267:TYR:HB2	1:C:296:TYR:CE2	2.53	0.43
1:A:135:ASN:OD1	1:E:64:LEU:HD12	2.18	0.43
1:B:331:LEU:HD12	1:B:335:PHE:CD2	2.53	0.43
1:C:154:ILE:HD13	1:D:133:LYS:HD2	2.00	0.43
1:C:25:VAL:HG11	1:C:191:GLY:HA3	2.01	0.43
1:A:51:MSE:N	1:A:120:ILE:O	2.52	0.43
1:C:61:ILE:HD11	1:C:124:ILE:O	2.18	0.43
1:E:61:ILE:HG23	1:E:66:LYS:HE3	2.01	0.43
1:A:64:LEU:HA	1:B:131:HIS:HD2	1.84	0.43
1:A:44:LEU:HD23	1:A:120:ILE:HB	2.00	0.43
1:B:341:LEU:O	1:B:344:GLN:O	2.37	0.42
1:C:214:PHE:CE2	1:C:221:CYS:SG	3.13	0.42
1:D:341:LEU:O	1:D:344:GLN:O	2.37	0.42
1:B:37:THR:HG22	1:B:74:MSE:HE1	2.00	0.42
1:C:28:ARG:NH2	1:D:170:ASN:OD1	2.53	0.42
1:D:331:LEU:HD12	1:D:331:LEU:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:VAL:HG23	1:E:312:PHE:O	2.20	0.42
1:E:177:ARG:O	1:E:177:ARG:HG3	2.20	0.42
1:D:9:TRP:O	1:D:35:ASN:OD1	2.38	0.41
1:E:26:GLY:HA3	1:E:225:VAL:O	2.20	0.41
1:C:65:GLU:HG2	1:D:135:ASN:ND2	2.35	0.41
1:D:94:ILE:CD1	1:D:107:LYS:HE2	2.49	0.41
1:E:57:LEU:HB2	1:E:60:GLU:HG3	2.01	0.41
1:C:51:MSE:CE	1:C:144:VAL:HG21	2.51	0.41
1:D:40:ALA:HB1	1:D:44:LEU:HD11	2.03	0.41
1:D:275:VAL:HG23	1:D:312:PHE:O	2.20	0.41
1:D:40:ALA:HB1	1:D:44:LEU:CD1	2.51	0.41
1:E:214:PHE:CE2	1:E:221:CYS:SG	3.14	0.41
1:C:51:MSE:HE2	1:C:144:VAL:HG21	2.02	0.41
1:C:260:ARG:NH2	1:C:343:GLN:O	2.53	0.41
1:D:10:THR:OG1	1:D:11:PRO:HD2	2.20	0.41
1:A:107:LYS:HD3	1:A:109:ILE:HD11	2.03	0.41
1:A:9:TRP:HZ3	1:A:36:VAL:HG23	1.86	0.40
1:C:41:LEU:HD11	1:C:74:MSE:CE	2.52	0.40
1:B:206:THR:HG23	1:B:209:ASP:H	1.86	0.40
1:C:57:LEU:HB2	1:C:60:GLU:HG3	2.03	0.40
1:C:261:THR:O	1:C:345:ASN:ND2	2.53	0.40
1:D:313:ASN:OD1	1:D:315:ASN:O	2.38	0.40
1:B:265:LYS:HB2	1:B:348:TYR:CD1	2.56	0.40
1:C:71:THR:HG22	1:C:72:GLU:N	2.36	0.40
1:A:331:LEU:HD12	1:A:331:LEU:C	2.41	0.40
1:B:326:LEU:HD23	1:B:331:LEU:HD13	2.04	0.40
1:D:44:LEU:HD23	1:D:120:ILE:HB	2.02	0.40
1:D:132:VAL:HB	1:D:135:ASN:ND2	2.36	0.40
1:E:27:GLY:N	1:E:225:VAL:O	2.54	0.40
1:A:313:ASN:OD1	1:A:315:ASN:O	2.39	0.40
1:E:134:SER:OG	1:E:174:THR:HA	2.21	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	362/374 (97%)	353 (98%)	9 (2%)	0	100	100
1	B	358/374 (96%)	350 (98%)	7 (2%)	1 (0%)	41	71
1	C	360/374 (96%)	353 (98%)	7 (2%)	0	100	100
1	D	359/374 (96%)	350 (98%)	9 (2%)	0	100	100
1	E	359/374 (96%)	353 (98%)	6 (2%)	0	100	100
All	All	1798/1870 (96%)	1759 (98%)	38 (2%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	VAL

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	324/335 (97%)	320 (99%)	4 (1%)	71	91
1	B	320/335 (96%)	317 (99%)	3 (1%)	78	93
1	C	325/335 (97%)	320 (98%)	5 (2%)	65	87
1	D	326/335 (97%)	322 (99%)	4 (1%)	71	91
1	E	327/335 (98%)	322 (98%)	5 (2%)	65	87
All	All	1622/1675 (97%)	1601 (99%)	21 (1%)	69	90

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	48	ASN
1	A	127	SER
1	A	145	PHE

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Mol	Chain	Res	Type
1	B	43	ASP
1	B	127	SER
1	B	145	PHE
1	C	43	ASP
1	C	48	ASN
1	C	127	SER
1	C	145	PHE
1	C	227	ASN
1	D	43	ASP
1	D	48	ASN
1	D	127	SER
1	D	145	PHE
1	E	43	ASP
1	E	48	ASN
1	E	127	SER
1	E	145	PHE
1	E	227	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	B	131	HIS
1	B	170	ASN
1	D	67	ASN
1	E	170	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	500	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	D	500	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	E	500	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	500	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	500	-	4,4,4	0.14	0	6,6,6	0.05	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	SO4	1	0

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	356/374 (95%)	0.26	11 (3%) 49 44	29, 51, 100, 152	0
1	B	352/374 (94%)	0.33	9 (2%) 56 52	30, 49, 88, 116	0
1	C	354/374 (94%)	0.21	15 (4%) 36 32	23, 45, 83, 136	0
1	D	353/374 (94%)	0.36	19 (5%) 25 22	28, 55, 100, 138	0
1	E	353/374 (94%)	0.30	16 (4%) 33 29	30, 50, 98, 127	0
All	All	1768/1870 (94%)	0.29	70 (3%) 38 33	23, 50, 95, 152	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	229	GLN	8.2
1	C	7	GLU	6.9
1	E	229	GLN	5.6
1	B	79	PHE	5.0
1	E	134	SER	4.5
1	A	326	LEU	4.4
1	D	230	GLU	4.4
1	D	229	GLN	3.8
1	A	229	GLN	3.8
1	E	326	LEU	3.7
1	A	132	VAL	3.6
1	A	368	GLU	3.5
1	B	326	LEU	3.5
1	B	335	PHE	3.5
1	C	8	PHE	3.5
1	D	86	PHE	3.3
1	A	225	VAL	3.2
1	C	157	ASN	3.1
1	E	227	ASN	3.1
1	C	156	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	230	GLU	3.0
1	D	87	ASN	3.0
1	E	274	LEU	3.0
1	D	84	SER	3.0
1	B	142	TYR	3.0
1	A	9	TRP	3.0
1	C	154	ILE	2.8
1	D	103	ILE	2.8
1	C	30	VAL	2.7
1	D	175	ILE	2.7
1	A	156	PRO	2.7
1	B	282	LEU	2.6
1	A	329	THR	2.6
1	E	329	THR	2.6
1	C	158	ALA	2.6
1	A	7	GLU	2.5
1	E	225	VAL	2.5
1	D	156	PRO	2.5
1	C	291	SER	2.5
1	E	330	GLN	2.5
1	B	367	LEU	2.5
1	E	135	ASN	2.4
1	D	133	LYS	2.4
1	D	79	PHE	2.4
1	C	27	GLY	2.4
1	D	326	LEU	2.4
1	A	131	HIS	2.4
1	E	154	ILE	2.3
1	B	339	PHE	2.3
1	B	341	LEU	2.3
1	D	332	LYS	2.3
1	C	211	LYS	2.3
1	E	328	GLU	2.3
1	E	178	LYS	2.3
1	C	252	LYS	2.3
1	D	83	PHE	2.2
1	D	99	ILE	2.2
1	D	130	GLY	2.2
1	E	158	ALA	2.2
1	A	49	VAL	2.2
1	C	232	LEU	2.2
1	E	228	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	228	LYS	2.2
1	B	120	ILE	2.2
1	C	9	TRP	2.1
1	D	274	LEU	2.1
1	D	178	LYS	2.1
1	D	89	ASP	2.1
1	E	152	ARG	2.1
1	D	81	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 monosaccharides 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, 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	B-factors(\AA^2)	Q<0.9
2	SO4	E	500	5/5	0.61	0.37	115,120,129,161	0
2	SO4	B	500	5/5	0.78	0.28	81,87,104,107	0
2	SO4	C	500	5/5	0.85	0.20	91,91,111,123	0
2	SO4	A	500	5/5	0.92	0.16	72,77,86,93	0
2	SO4	D	500	5/5	0.96	0.20	50,60,66,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.