



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:35 AM GMT

PDB ID : 3IXS
Title : Ring1B C-terminal domain/RYBP C-terminal domain Complex
Authors : Wang, R.; Taylor, A.B.; Kim, C.A.
Deposited on : 2009-09-04
Resolution : 1.70 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

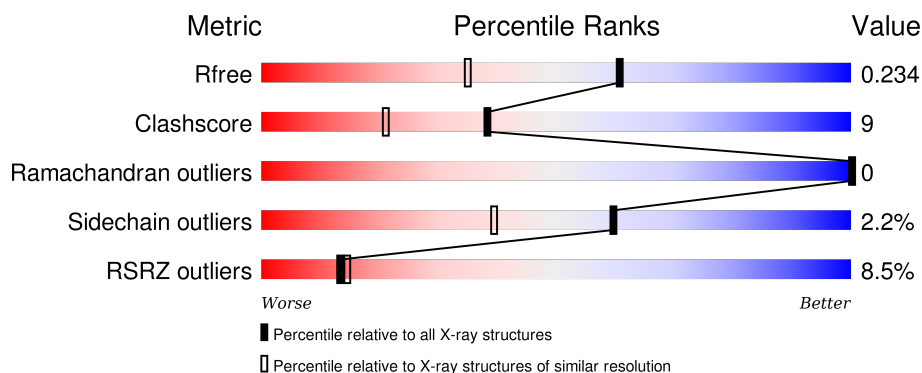
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	111	<div> <div>3%</div> <div>86%</div> <div>14%</div> <div>•</div> </div>
1	C	111	<div> <div>5%</div> <div>83%</div> <div>17%</div> </div>
1	E	111	<div> <div>5%</div> <div>72%</div> <div>19%</div> <div>9%</div> </div>
1	G	111	<div> <div>9%</div> <div>67%</div> <div>22%</div> <div>•</div> <div>11%</div> </div>
1	I	111	<div> <div>13%</div> <div>73%</div> <div>13%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	111	
2	B	37	
2	D	37	
2	F	37	
2	H	37	
2	J	37	
2	L	37	

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	EDO	C	4	-	-	X	X
3	EDO	E	1	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6935 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 E3 ubiquitin-protein ligase RING2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	1	0
			890	564	145	178	3			
1	C	111	Total	C	N	O	S	0	2	0
			893	566	145	179	3			
1	E	101	Total	C	N	O	S	0	0	0
			810	519	130	159	2			
1	G	99	Total	C	N	O	S	0	1	0
			798	512	129	155	2			
1	I	95	Total	C	N	O	S	0	0	0
			766	493	123	148	2			
1	K	100	Total	C	N	O	S	0	0	0
			803	514	130	157	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	ASP	ASN	ENGINEERED	UNP Q99496
C	306	ASP	ASN	ENGINEERED	UNP Q99496
E	306	ASP	ASN	ENGINEERED	UNP Q99496
G	306	ASP	ASN	ENGINEERED	UNP Q99496
I	306	ASP	ASN	ENGINEERED	UNP Q99496
K	306	ASP	ASN	ENGINEERED	UNP Q99496

- Molecule 2 is a protein called RING1 and YY1-binding protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	31	Total	C	N	O	0	0	0
			241	151	44	46			
2	D	34	Total	C	N	O	0	0	0
			263	163	50	50			
2	F	32	Total	C	N	O	0	0	0
			252	157	48	47			

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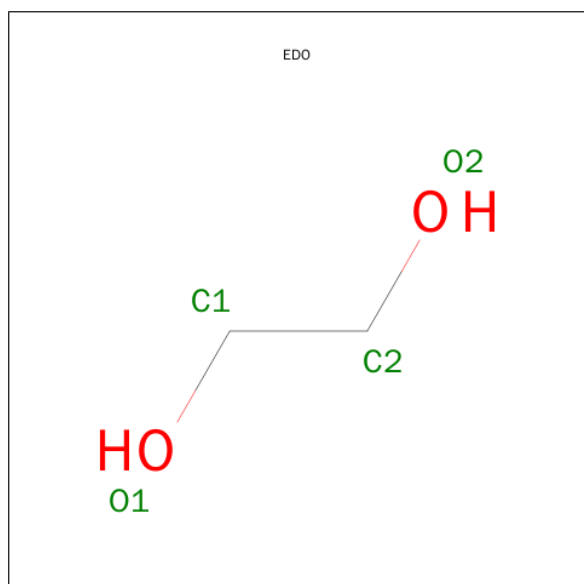
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	36	Total	C	N	O	0	0	0
			283	174	55	54			
2	J	30	Total	C	N	O	0	0	0
			234	146	43	45			
2	L	32	Total	C	N	O	0	0	0
			252	157	48	47			

There are 12 discrepancies between the modelled and reference sequences:

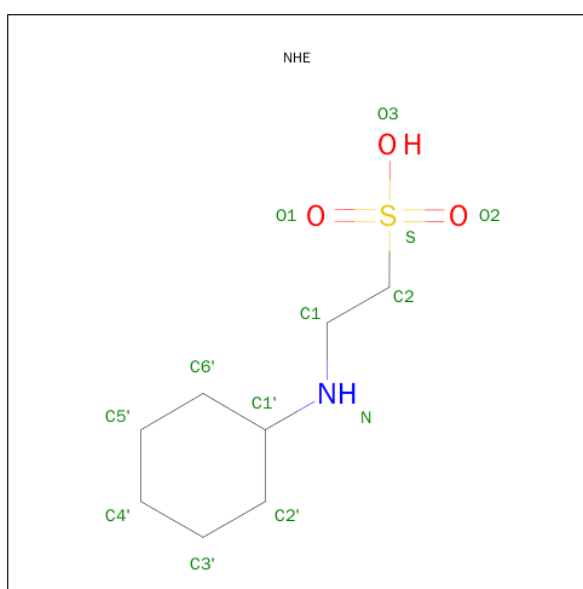
Chain	Residue	Modelled	Actual	Comment	Reference
B	143	GLY	-	EXPRESSION TAG	UNP Q8N488
B	144	THR	-	EXPRESSION TAG	UNP Q8N488
D	143	GLY	-	EXPRESSION TAG	UNP Q8N488
D	144	THR	-	EXPRESSION TAG	UNP Q8N488
F	143	GLY	-	EXPRESSION TAG	UNP Q8N488
F	144	THR	-	EXPRESSION TAG	UNP Q8N488
H	143	GLY	-	EXPRESSION TAG	UNP Q8N488
H	144	THR	-	EXPRESSION TAG	UNP Q8N488
J	143	GLY	-	EXPRESSION TAG	UNP Q8N488
J	144	THR	-	EXPRESSION TAG	UNP Q8N488
L	143	GLY	-	EXPRESSION TAG	UNP Q8N488
L	144	THR	-	EXPRESSION TAG	UNP Q8N488

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O S 13 8 1 3 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	88	Total O 88 88	0	0
5	B	27	Total O 27 27	0	0
5	C	100	Total O 100 100	0	0
5	D	36	Total O 36 36	0	0

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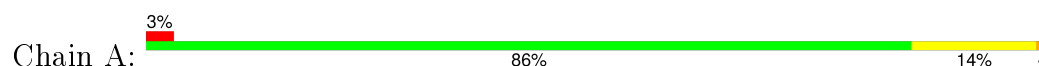
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	53	Total 53	O 53	0	0
5	F	12	Total 12	O 12	0	0
5	G	24	Total 24	O 24	0	0
5	H	13	Total 13	O 13	0	0
5	I	16	Total 16	O 16	0	0
5	J	9	Total 9	O 9	0	0
5	K	36	Total 36	O 36	0	0
5	L	7	Total 7	O 7	0	0

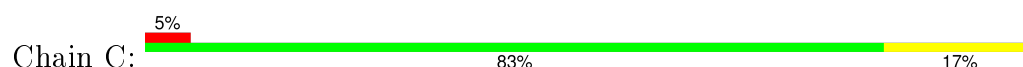
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

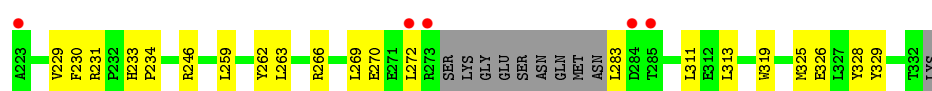
- Molecule 1: E3 ubiquitin-protein ligase RING2



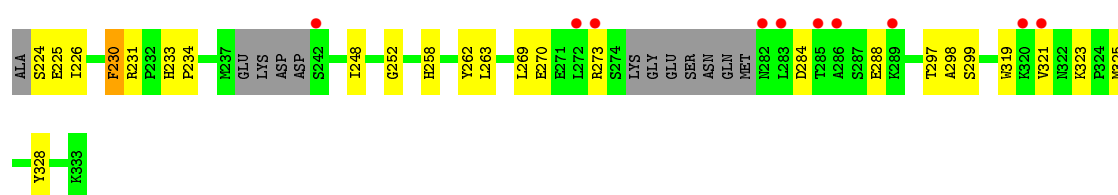
- Molecule 1: E3 ubiquitin-protein ligase RING2



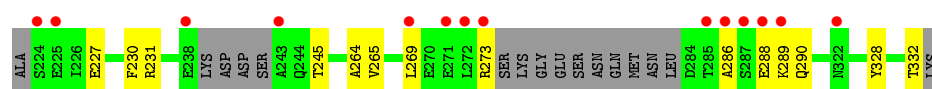
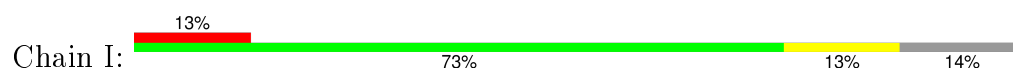
- Molecule 1: E3 ubiquitin-protein ligase RING2



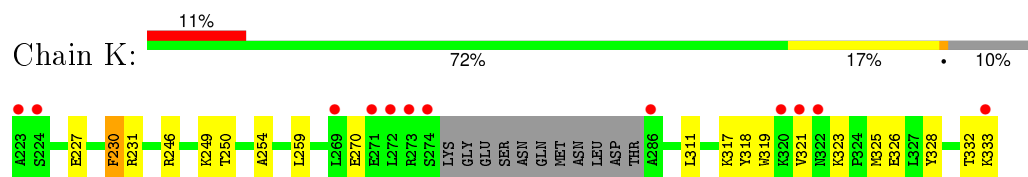
- Molecule 1: E3 ubiquitin-protein ligase RING2



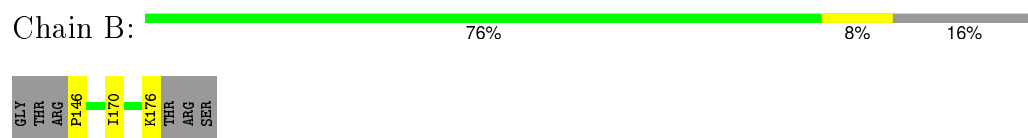
- Molecule 1: E3 ubiquitin-protein ligase RING2



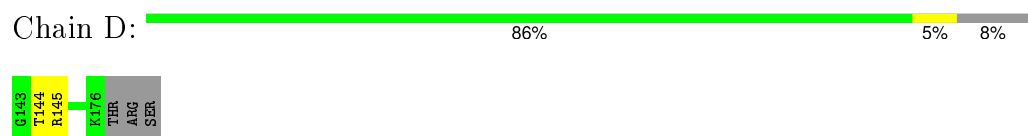
- Molecule 1: E3 ubiquitin-protein ligase RING2



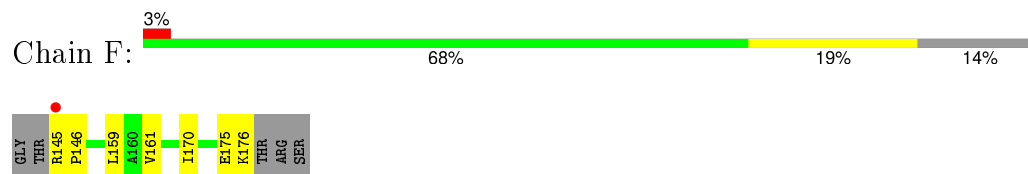
- Molecule 2: RING1 and YY1-binding protein



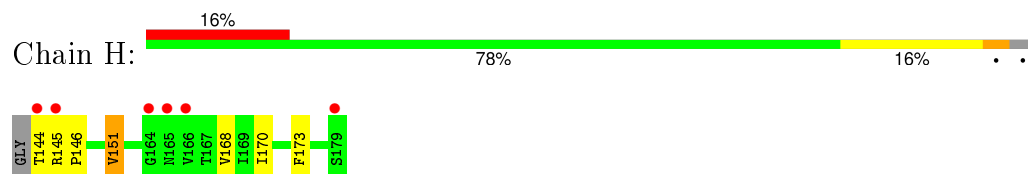
- Molecule 2: RING1 and YY1-binding protein



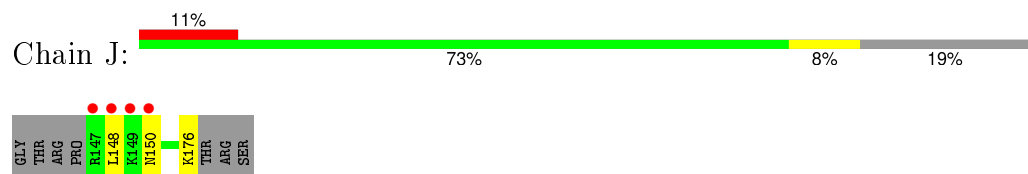
- Molecule 2: RING1 and YY1-binding protein



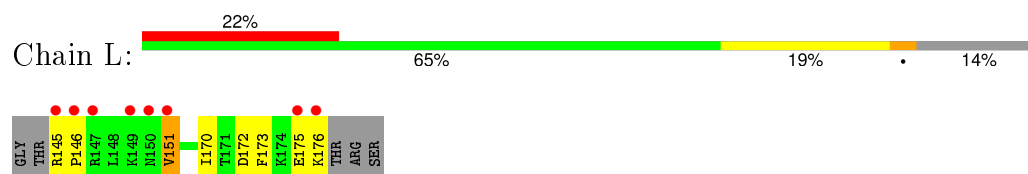
- Molecule 2: RING1 and YY1-binding protein



- Molecule 2: RING1 and YY1-binding protein



- Molecule 2: RING1 and YY1-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	37.89Å 56.55Å 100.35Å 100.88° 90.61° 100.49°	Depositor
Resolution (Å)	40.68 – 1.70 40.68 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.9 (40.68-1.70) 90.1 (40.68-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_4)	Depositor
R, R_{free}	0.203 , 0.234 0.202 , 0.234	Depositor DCC
R_{free} test set	4271 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 84786 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6935	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NHE, EDO

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	0.37	0/910	0.60	0/1229
1	C	0.41	0/916	0.60	0/1237
1	E	0.32	0/826	0.53	0/1119
1	G	0.29	0/816	0.48	0/1102
1	I	0.26	0/781	0.45	0/1057
1	K	0.33	0/819	0.52	0/1106
2	B	0.43	0/242	0.65	0/326
2	D	0.43	0/264	0.66	0/356
2	F	0.30	0/253	0.56	0/341
2	H	0.32	0/284	0.55	0/383
2	J	0.29	0/234	0.53	0/315
2	L	0.27	0/253	0.49	0/341
All	All	0.34	0/6598	0.55	0/8912

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	890	0	883	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	893	0	888	14	0
1	E	810	0	803	21	0
1	G	798	0	799	22	0
1	I	766	0	760	8	0
1	K	803	0	799	17	0
2	B	241	0	258	3	0
2	D	263	0	280	2	0
2	F	252	0	270	11	0
2	H	283	0	302	11	0
2	J	234	0	250	2	0
2	L	252	0	270	7	0
3	A	4	0	6	0	0
3	C	4	0	6	4	0
3	E	4	0	6	4	0
3	H	4	0	6	0	0
4	C	13	0	17	0	0
5	A	88	0	0	1	0
5	B	27	0	0	0	0
5	C	100	0	0	3	0
5	D	36	0	0	0	0
5	E	53	0	0	1	0
5	F	12	0	0	0	0
5	G	24	0	0	0	0
5	H	13	0	0	0	0
5	I	16	0	0	0	0
5	J	9	0	0	0	0
5	K	36	0	0	0	0
5	L	7	0	0	0	0
All	All	6935	0	6603	119	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 9.

All (119) 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:E:246:ARG:HE	3:E:1:EDO:H12	1.09	1.07
1:K:231:ARG:HH12	1:K:326:GLU:CD	1.71	0.93
1:A:332:THR:HA	1:A:333:LYS:CB	2.01	0.90
3:C:4:EDO:H21	2:D:145:ARG:HG3	1.56	0.87
2:F:175:GLU:O	2:F:176:LYS:HB2	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:THR:HA	1:A:333:LYS:HB2	1.66	0.76
1:E:246:ARG:NE	3:E:1:EDO:H12	1.95	0.74
3:C:4:EDO:H11	5:C:1153:HOH:O	1.87	0.74
2:H:151:VAL:CG2	2:H:173:PHE:HB2	2.18	0.74
1:K:227:GLU:HG2	1:K:249:LYS:HB3	1.71	0.72
2:J:150:ASN:OD1	2:J:176:LYS:HB2	1.90	0.71
1:A:332:THR:HA	1:A:333:LYS:HB3	1.70	0.71
1:G:226:ILE:HG13	2:H:145:ARG:HD3	1.72	0.70
1:G:226:ILE:HD13	1:G:252:GLY:HA2	1.74	0.70
1:C:242:SER:HB3	1:C:244:GLN:HB2	1.74	0.69
2:L:145:ARG:N	2:L:146:PRO:HD3	2.09	0.68
1:G:226:ILE:HD13	1:G:252:GLY:CA	2.24	0.67
1:A:332:THR:CA	1:A:333:LYS:CB	2.73	0.65
1:C:243:ALA:HA	5:C:1171:HOH:O	1.96	0.65
1:E:266:ARG:HH21	2:F:159:LEU:HD23	1.62	0.64
1:G:297:THR:HG22	1:G:299:SER:H	1.64	0.63
1:G:269:LEU:O	1:G:273:ARG:HG3	1.99	0.63
2:H:151:VAL:HG22	2:H:173:PHE:HB2	1.80	0.63
1:E:263:LEU:HD22	3:E:1:EDO:H11	1.82	0.62
1:A:333:LYS:OXT	1:A:333:LYS:HG2	2.00	0.61
1:I:264:ALA:HB1	1:I:286:ALA:HB1	1.83	0.61
1:A:332:THR:CA	1:A:333:LYS:HB3	2.30	0.60
1:C:226:ILE:HA	3:C:4:EDO:H22	1.83	0.60
1:A:253:ASN:HB2	5:A:1069:HOH:O	2.01	0.60
2:H:151:VAL:HG21	2:H:173:PHE:HB2	1.82	0.59
1:E:319:TRP:CD1	1:E:325:MET:HG2	2.37	0.59
1:G:225:GLU:O	2:H:145:ARG:HD2	2.02	0.59
1:E:272:LEU:O	1:E:272:LEU:HD12	2.03	0.59
2:F:145:ARG:HB3	2:F:146:PRO:HA	1.85	0.58
1:G:225:GLU:C	1:G:226:ILE:HD12	2.24	0.58
1:G:224:SER:HB2	2:H:145:ARG:HE	1.70	0.57
1:E:266:ARG:NH2	2:F:159:LEU:HD23	2.19	0.56
2:L:151:VAL:HG23	2:L:173:PHE:HB3	1.88	0.55
1:G:319:TRP:CG	1:G:325:MET:HG2	2.41	0.55
2:D:144:THR:O	2:D:144:THR:HG23	2.07	0.55
1:K:254:ALA:O	1:K:311:LEU:HD13	2.07	0.55
1:C:244:GLN:HB3	5:C:1213:HOH:O	2.05	0.55
1:E:266:ARG:O	1:E:270:GLU:HG3	2.06	0.55
1:G:270:GLU:HA	1:G:273:ARG:HD2	1.89	0.55
1:C:321:VAL:HG11	1:C:323:LYS:HE2	1.88	0.55
1:G:226:ILE:HD12	1:G:226:ILE:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:SER:HB3	1:A:249:LYS:HD2	1.90	0.53
2:L:175:GLU:HG2	2:L:176:LYS:H	1.74	0.53
1:C:263:LEU:HD21	1:C:329:TYR:CD1	2.44	0.53
1:A:275:LYS:HB3	1:A:277:GLU:OE2	2.08	0.53
1:K:231:ARG:NH1	1:K:326:GLU:CD	2.53	0.52
2:F:159:LEU:HD12	2:F:161:VAL:HG23	1.93	0.51
1:I:290:GLN:O	1:I:332:THR:HG22	2.11	0.51
1:K:332:THR:O	1:K:333:LYS:OXT	2.29	0.51
1:G:231:ARG:O	1:G:328:TYR:HA	2.11	0.51
1:G:262:TYR:HB2	2:H:170:ILE:HD12	1.92	0.51
1:A:313:LEU:C	1:A:313:LEU:HD23	2.31	0.50
1:E:262:TYR:HD2	2:F:159:LEU:HD11	1.76	0.50
1:K:227:GLU:HG2	1:K:249:LYS:CB	2.40	0.49
1:C:225:GLU:O	3:C:4:EDO:H12	2.12	0.49
1:A:223:ALA:O	1:A:224:SER:HB2	2.12	0.49
1:E:231:ARG:O	1:E:328:TYR:HA	2.12	0.49
1:E:319:TRP:CG	1:E:325:MET:HG2	2.48	0.48
1:C:244:GLN:HA	1:C:244:GLN:OE1	2.13	0.48
1:A:262:TYR:HB2	2:B:170:ILE:HD12	1.94	0.48
1:C:231:ARG:O	1:C:328:TYR:HA	2.13	0.48
1:I:289:LYS:O	1:I:332:THR:HG21	2.14	0.48
1:K:250:THR:CB	2:L:170:ILE:HD13	2.44	0.47
1:C:239:LYS:O	1:C:239:LYS:HG3	2.14	0.47
1:E:262:TYR:CE2	2:F:159:LEU:HD21	2.48	0.47
1:G:258:HIS:CD2	2:H:168:VAL:HG22	2.49	0.47
5:E:1284:HOH:O	2:F:145:ARG:HB2	2.14	0.47
2:H:145:ARG:HA	2:H:146:PRO:HD3	1.73	0.46
1:E:262:TYR:HB2	2:F:170:ILE:CD1	2.45	0.46
1:I:231:ARG:O	1:I:328:TYR:HA	2.15	0.46
1:K:230:PHE:HZ	1:K:259:LEU:HB3	1.81	0.45
2:H:151:VAL:HG22	2:H:173:PHE:CB	2.46	0.45
1:I:269:LEU:O	1:I:273:ARG:HG2	2.16	0.45
1:E:259:LEU:HD21	1:E:311:LEU:HD11	1.98	0.45
1:G:224:SER:CB	2:H:145:ARG:HE	2.28	0.45
1:E:231:ARG:HH12	1:E:326:GLU:CD	2.21	0.44
1:I:227:GLU:HB3	2:J:148:LEU:HG	1.99	0.44
1:C:241:ASP:HA	1:C:242:SER:HA	1.49	0.44
1:K:317:LYS:HE2	1:K:318:TYR:CZ	2.53	0.44
1:E:262:TYR:HB2	2:F:170:ILE:HD13	1.99	0.44
1:I:264:ALA:CB	1:I:286:ALA:HB1	2.47	0.44
1:A:323:LYS:CA	2:B:146:PRO:HB3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:319:TRP:CE2	1:K:325:MET:HA	2.53	0.44
1:A:224:SER:HB3	1:A:249:LYS:CD	2.47	0.44
1:K:246:ARG:HH22	1:K:270:GLU:CD	2.21	0.44
1:I:265:VAL:O	1:I:269:LEU:HD13	2.18	0.43
1:G:321:VAL:HG12	1:G:323:LYS:HG2	1.99	0.43
1:E:329:TYR:CZ	3:E:1:EDO:H22	2.53	0.43
1:A:332:THR:CB	1:A:333:LYS:HB3	2.48	0.43
1:K:250:THR:HB	2:L:170:ILE:HD13	2.01	0.43
1:A:265:VAL:HG13	1:A:283:LEU:HD11	2.00	0.43
2:B:176:LYS:HE2	2:B:176:LYS:HB3	1.82	0.42
2:F:175:GLU:O	2:F:176:LYS:CB	2.56	0.42
1:C:263:LEU:HD21	1:C:329:TYR:CG	2.55	0.42
1:E:269:LEU:HD21	1:E:283:LEU:HD11	2.01	0.42
1:A:231:ARG:O	1:A:328:TYR:HA	2.19	0.42
1:K:230:PHE:CZ	1:K:259:LEU:HB3	2.53	0.42
1:E:313:LEU:C	1:E:313:LEU:HD23	2.40	0.42
1:K:321:VAL:HG21	1:K:323:LYS:HE2	2.02	0.42
1:K:321:VAL:CG2	1:K:323:LYS:HG2	2.50	0.41
1:K:321:VAL:HG23	1:K:323:LYS:HG2	2.01	0.41
1:G:230:PHE:CZ	1:G:263:LEU:HD11	2.55	0.41
1:G:319:TRP:CD1	1:G:325:MET:HG2	2.55	0.41
2:L:175:GLU:HG2	2:L:176:LYS:N	2.35	0.41
1:G:248:ILE:HD11	1:G:262:TYR:OH	2.21	0.41
1:G:233:HIS:HA	1:G:234:PRO:HD3	1.85	0.41
1:G:288:GLU:H	1:G:288:GLU:CD	2.24	0.41
1:K:231:ARG:O	1:K:328:TYR:HA	2.20	0.41
2:L:145:ARG:N	2:L:146:PRO:CD	2.79	0.41
1:E:233:HIS:HA	1:E:234:PRO:HD3	1.85	0.41
1:G:297:THR:HG22	1:G:298:ALA:N	2.36	0.41
1:C:294:TYR:CE2	1:C:304:VAL:HG22	2.56	0.41
1:E:229:VAL:CG1	1:E:326:GLU:HG2	2.51	0.40
1:C:317:LYS:HE3	1:C:317:LYS:HB3	1.81	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	110/111 (99%)	107 (97%)	3 (3%)	0	100	100
1	C	111/111 (100%)	108 (97%)	3 (3%)	0	100	100
1	E	97/111 (87%)	94 (97%)	3 (3%)	0	100	100
1	G	94/111 (85%)	90 (96%)	4 (4%)	0	100	100
1	I	89/111 (80%)	87 (98%)	2 (2%)	0	100	100
1	K	96/111 (86%)	93 (97%)	3 (3%)	0	100	100
2	B	29/37 (78%)	29 (100%)	0	0	100	100
2	D	32/37 (86%)	32 (100%)	0	0	100	100
2	F	30/37 (81%)	28 (93%)	2 (7%)	0	100	100
2	H	34/37 (92%)	34 (100%)	0	0	100	100
2	J	28/37 (76%)	28 (100%)	0	0	100	100
2	L	30/37 (81%)	28 (93%)	2 (7%)	0	100	100
All	All	780/888 (88%)	758 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	99/98 (101%)	97 (98%)	2 (2%)	63	44
1	C	100/98 (102%)	97 (97%)	3 (3%)	48	26
1	E	89/98 (91%)	88 (99%)	1 (1%)	80	69
1	G	89/98 (91%)	87 (98%)	2 (2%)	60	39
1	I	84/98 (86%)	81 (96%)	3 (4%)	42	19
1	K	88/98 (90%)	87 (99%)	1 (1%)	80	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	28/33 (85%)	28 (100%)	0	100	100
2	D	30/33 (91%)	30 (100%)	0	100	100
2	F	29/33 (88%)	29 (100%)	0	100	100
2	H	33/33 (100%)	31 (94%)	2 (6%)	23	7
2	J	27/33 (82%)	27 (100%)	0	100	100
2	L	29/33 (88%)	27 (93%)	2 (7%)	19	5
All	All	725/786 (92%)	709 (98%)	16 (2%)	60	39

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	SER
1	A	230	PHE
1	C	240	ASP
1	C	262	TYR
1	C	287	SER
1	E	230	PHE
1	G	230	PHE
1	G	284	ASP
2	H	144	THR
2	H	151	VAL
1	I	230	PHE
1	I	245	THR
1	I	288	GLU
1	K	230	PHE
2	L	151	VAL
2	L	172	ASP

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 [i](#)

There are no carbohydrates 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	$\# Z > 2$
3	EDO	A	2	-	3,3,3	0.53	0	2,2,2	0.37	0
4	NHE	C	1	-	12,13,13	3.01	3 (25%)	15,17,17	1.31	1 (6%)
3	EDO	C	4	-	3,3,3	0.49	0	2,2,2	0.48	0
3	EDO	E	1	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	H	3	-	3,3,3	0.47	0	2,2,2	0.37	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	EDO	A	2	-	-	0/1/1/1	0/0/0/0
4	NHE	C	1	-	-	0/7/15/15	0/1/1/1
3	EDO	C	4	-	-	0/1/1/1	0/0/0/0
3	EDO	E	1	-	-	0/1/1/1	0/0/0/0
3	EDO	H	3	-	-	0/1/1/1	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NHE	O1-S	4.33	1.58	1.45
4	C	1	NHE	O2-S	6.22	1.64	1.45
4	C	1	NHE	O3-S	6.47	1.63	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	C	1	NHE	O1-S-C2	4.21	110.49	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	EDO	4	0
3	E	1	EDO	4	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	111/111 (100%)	0.18	3 (2%) 58 62	15, 26, 44, 52	0
1	C	111/111 (100%)	0.26	6 (5%) 29 31	16, 22, 56, 77	0
1	E	101/111 (90%)	0.29	5 (4%) 32 35	22, 32, 56, 80	0
1	G	99/111 (89%)	0.47	10 (10%) 9 9	23, 34, 62, 67	0
1	I	95/111 (85%)	0.74	14 (14%) 3 4	28, 38, 67, 82	0
1	K	100/111 (90%)	0.63	12 (12%) 6 6	17, 32, 64, 85	0
2	B	31/37 (83%)	0.34	0 100 100	14, 20, 44, 50	0
2	D	34/37 (91%)	0.26	0 100 100	16, 21, 41, 47	0
2	F	32/37 (86%)	0.25	1 (3%) 52 57	27, 41, 53, 55	0
2	H	36/37 (97%)	0.53	6 (16%) 2 2	26, 35, 57, 58	0
2	J	30/37 (81%)	0.73	4 (13%) 4 5	28, 42, 59, 60	0
2	L	32/37 (86%)	0.99	8 (25%) 1 1	25, 48, 68, 69	0
All	All	812/888 (91%)	0.44	69 (8%) 13 14	14, 32, 61, 85	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	321	VAL	9.2
1	I	286	ALA	8.8
1	E	272	LEU	7.6
1	I	272	LEU	7.5
1	G	273	ARG	7.4
1	K	273	ARG	7.2
1	K	274	SER	6.9
1	C	242	SER	6.3
1	G	272	LEU	6.0
1	I	285	THR	5.9
1	E	273	ARG	5.8

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Mol	Chain	Res	Type	RSRZ
1	E	285	THR	5.3
1	C	239	LYS	5.0
2	H	165	ASN	5.0
1	A	223	ALA	4.9
2	H	144	THR	4.9
1	I	271	GLU	4.9
1	K	272	LEU	4.5
1	K	223	ALA	4.4
1	K	286	ALA	4.3
1	A	333	LYS	4.2
2	F	145	ARG	4.2
2	L	146	PRO	4.1
2	L	145	ARG	4.0
1	K	271	GLU	4.0
2	H	179	SER	4.0
1	I	243	ALA	3.9
1	K	224	SER	3.8
1	G	282	ASN	3.7
1	C	241	ASP	3.7
1	I	273	ARG	3.5
1	I	289	LYS	3.4
2	J	150	ASN	3.4
1	I	269	LEU	3.4
1	G	286	ALA	3.4
1	I	288	GLU	3.3
1	G	242	SER	3.2
1	E	284	ASP	3.2
1	K	322	ASN	3.1
1	C	243	ALA	3.1
1	G	289	LYS	3.0
1	C	333	LYS	3.0
2	J	149	LYS	2.9
1	G	321	VAL	2.9
2	J	148	LEU	2.8
2	H	164	GLY	2.8
2	L	151	VAL	2.8
1	K	333	LYS	2.8
1	I	224	SER	2.8
1	I	322	ASN	2.7
1	K	269	LEU	2.7
1	I	287	SER	2.6
1	I	238	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	224	SER	2.5
2	L	176	LYS	2.5
1	G	320	LYS	2.5
1	K	320	LYS	2.5
2	H	166	VAL	2.4
2	L	149	LYS	2.4
2	L	147	ARG	2.3
1	C	240	ASP	2.3
1	E	223	ALA	2.2
2	L	175	GLU	2.2
1	I	225	GLU	2.1
2	H	145	ARG	2.1
2	J	147	ARG	2.1
2	L	150	ASN	2.0
1	G	283	LEU	2.0
1	G	285	THR	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	EDO	C	4	4/4	0.86	0.27	14.22	23,25,39,46	0
4	NHE	C	1	13/13	0.98	0.14	1.55	13,16,19,20	0
3	EDO	E	1	4/4	0.92	0.16	1.42	36,40,42,44	0
3	EDO	H	3	4/4	0.91	0.11	0.36	36,46,52,54	0
3	EDO	A	2	4/4	0.94	0.08	-0.94	19,23,25,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.