



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 08:33 PM UTC

PDB ID : 3IXS / pdb_00003ixs
Title : Ring1B C-terminal domain/RYPB 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

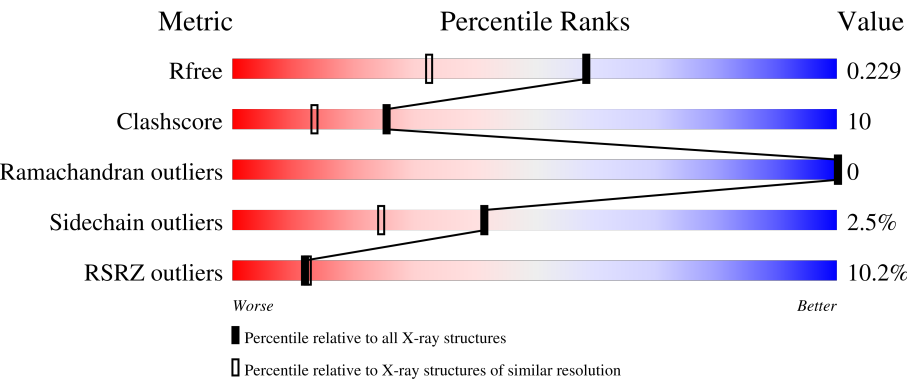
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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	111	8% 83%16%.
1	C	111	5% 83%16%.
1	E	111	6% 70%21%9%
1	G	111	14% 64%24%.11%
1	I	111	13% 70%15%14%

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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	-
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 mutation	UNP Q99496
C	306	ASP	ASN	engineered mutation	UNP Q99496
E	306	ASP	ASN	engineered mutation	UNP Q99496
G	306	ASP	ASN	engineered mutation	UNP Q99496
I	306	ASP	ASN	engineered mutation	UNP Q99496
K	306	ASP	ASN	engineered mutation	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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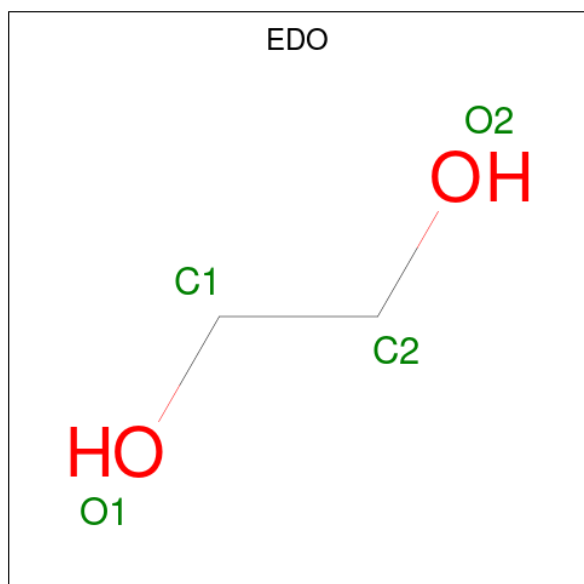
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	36	Total	C	N	O	0	0	0
			283	174	55	54			
2	J	30	Total	C	N	O	0	0	0
			234	146	43	45			
2	L	32	Total	C	N	O	0	0	0
			252	157	48	47			

There are 12 discrepancies between the modelled and reference sequences:

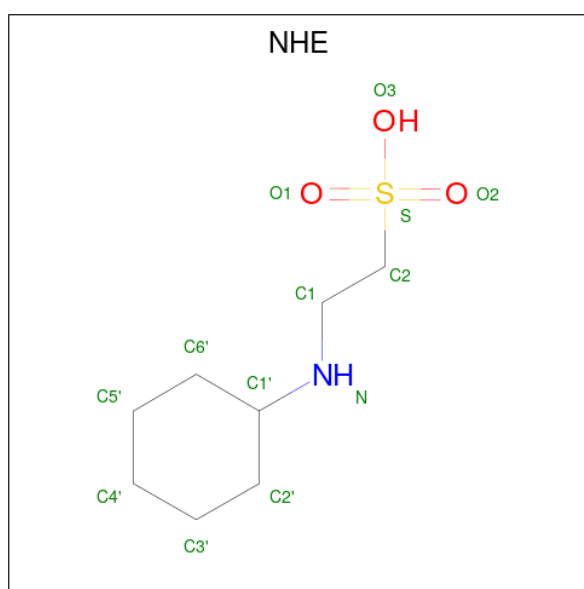
Chain	Residue	Modelled	Actual	Comment	Reference
B	143	GLY	-	expression tag	UNP Q8N488
B	144	THR	-	expression tag	UNP Q8N488
D	143	GLY	-	expression tag	UNP Q8N488
D	144	THR	-	expression tag	UNP Q8N488
F	143	GLY	-	expression tag	UNP Q8N488
F	144	THR	-	expression tag	UNP Q8N488
H	143	GLY	-	expression tag	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 (CCD ID: 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 (CCD ID: 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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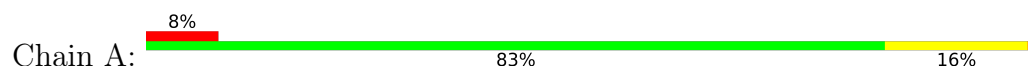
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	53	Total 53	O 53	0	0
5	F	12	Total 12	O 12	0	0
5	G	24	Total 24	O 24	0	0
5	H	13	Total 13	O 13	0	0
5	I	16	Total 16	O 16	0	0
5	J	9	Total 9	O 9	0	0
5	K	36	Total 36	O 36	0	0
5	L	7	Total 7	O 7	0	0

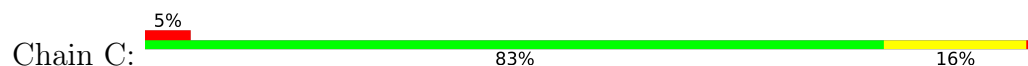
3 Residue-property plots

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.

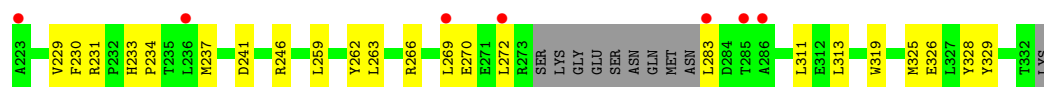
- Molecule 1: E3 ubiquitin-protein ligase RING2



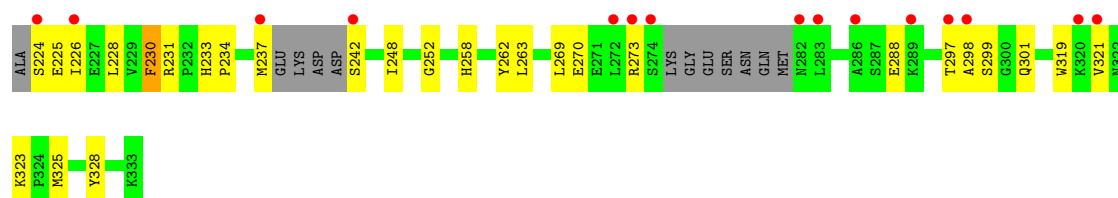
- Molecule 1: E3 ubiquitin-protein ligase RING2



- Molecule 1: E3 ubiquitin-protein ligase RING2

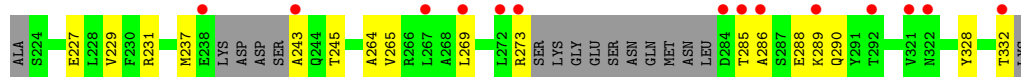


- Molecule 1: E3 ubiquitin-protein ligase RING2

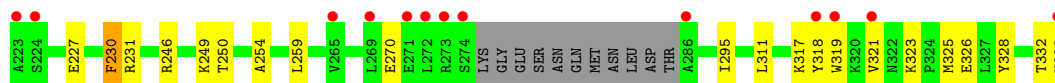


- Molecule 1: E3 ubiquitin-protein ligase RING2

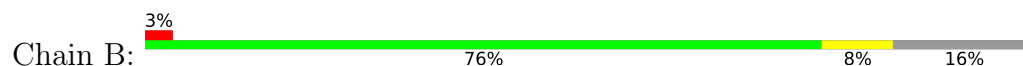




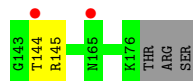
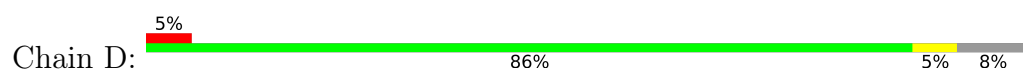
- Molecule 1: E3 ubiquitin-protein ligase RING2



- Molecule 2: RING1 and YY1-binding protein



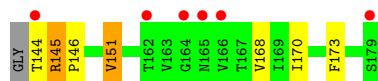
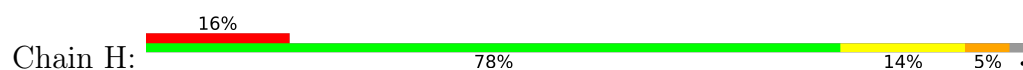
- Molecule 2: RING1 and YY1-binding protein



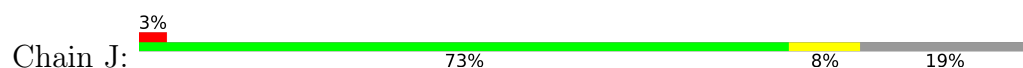
- Molecule 2: RING1 and YY1-binding protein



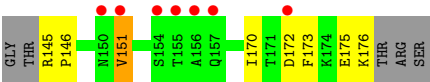
- Molecule 2: RING1 and YY1-binding protein



- 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) 95.9 (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 0.198 , 0.229	Depositor DCC
R_{free} test set	4271 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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: 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	0.45	0/910	0.80	0/1229
1	C	0.49	0/916	0.78	1/1237 (0.1%)
1	E	0.39	0/826	0.73	0/1119
1	G	0.35	0/816	0.71	0/1102
1	I	0.32	0/781	0.66	0/1057
1	K	0.39	0/819	0.70	0/1106
2	B	0.54	0/242	0.84	0/326
2	D	0.50	0/264	0.85	0/356
2	F	0.35	0/253	0.77	0/341
2	H	0.39	0/284	0.83	2/383 (0.5%)
2	J	0.32	0/234	0.71	0/315
2	L	0.34	0/253	0.72	0/341
All	All	0.41	0/6598	0.75	3/8912 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	145	ARG	CA-C-N	5.77	125.96	119.90
2	H	145	ARG	C-N-CA	5.77	125.96	119.90
1	C	321	VAL	N-CA-C	5.08	116.60	108.89

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	890	0	883	19	0
1	C	893	0	888	14	0
1	E	810	0	803	22	0
1	G	798	0	799	24	0
1	I	766	0	760	10	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	126	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 10.

All (126) 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	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:225:GLU:C	1:G:226:ILE:HD12	2.24	0.63
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:G:237:MET:HE1	1:G:242:SER:O	2.01	0.61
1:A:332:THR:CA	1:A:333:LYS:HB3	2.30	0.60
1:K:231:ARG:NH1	1:K:326:GLU:CD	2.53	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:HD12	1:E:272:LEU:O	2.03	0.59
2:F:145:ARG:HB3	2:F:146:PRO:HA	1.85	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:HG23	2:D:144:THR:O	2.07	0.55
1:K:254:ALA:O	1:K:311:LEU:HD13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:GLN:HB3	5:C:1213:HOH:O	2.05	0.55
1:A:313:LEU:C	1:A:313:LEU:HD23	2.31	0.55
1:C:321:VAL:HG11	1:C:323:LYS:HE2	1.88	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:G:226:ILE:HD12	1:G:226:ILE:N	2.22	0.55
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
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:264:ALA:HA	1:A:281:MET:HE3	1.94	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:E:231:ARG:HH12	1:E:326:GLU:CD	2.21	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:K:246:ARG:HH22	1:K:270:GLU:CD	2.21	0.48
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:C:239:LYS:O	1:C:239:LYS:HG3	2.14	0.47
1:I:237:MET:HE2	1:I:243:ALA:HB2	1.96	0.47
1:K:250:THR:CB	2:L:170:ILE:HD13	2.44	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
1:E:313:LEU:C	1:E:313:LEU:HD23	2.40	0.46
1:E:262:TYR:HB2	2:F:170:ILE:CD1	2.45	0.46
2:H:145:ARG:HA	2:H:146:PRO:HD3	1.73	0.46
1:I:231:ARG:O	1:I:328:TYR:HA	2.15	0.46
1:G:288:GLU:H	1:G:288:GLU:CD	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:G:228:LEU:HD12	1:G:228:LEU:C	2.43	0.44
1:G:321:VAL:HG12	1:G:323:LYS:HG2	1.99	0.43
1:I:265:VAL:O	1:I:269:LEU:HD13	2.18	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:HB3	2:B:176:LYS:HE2	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:K:321:VAL:HG21	1:K:323:LYS:HE2	2.02	0.42
1:A:267:LEU:HD23	1:A:281:MET:HE2	2.02	0.41
1:K:321:VAL:HG23	1:K:323:LYS:HG2	2.01	0.41
1:K:321:VAL:CG2	1:K:323:LYS:HG2	2.50	0.41
1:G:230:PHE:CZ	1:G:263:LEU:HD11	2.55	0.41
1:G:233:HIS:HA	1:G:234:PRO:HD3	1.85	0.41
1:G:248:ILE:HD11	1:G:262:TYR:OH	2.21	0.41
1:G:319:TRP:CD1	1:G:325:MET:HG2	2.55	0.41
1:I:285:THR:O	1:I:286:ALA:C	2.64	0.41
2:L:175:GLU:HG2	2:L:176:LYS:N	2.35	0.41
1:E:233:HIS:HA	1:E:234:PRO:HD3	1.85	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:C:294:TYR:CE2	1:C:304:VAL:HG22	2.56	0.41
1:G:297:THR:HG22	1:G:298:ALA:N	2.36	0.41
1:E:229:VAL:CG1	1:E:326:GLU:HG2	2.51	0.40
1:E:237:MET:HE3	1:E:241:ASP:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:LYS:HE3	1:C:317:LYS:HB3	1.81	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	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 [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	99/98 (101%)	97 (98%)	2 (2%)	48	32
1	C	100/98 (102%)	96 (96%)	4 (4%)	28	12
1	E	89/98 (91%)	88 (99%)	1 (1%)	65	54
1	G	89/98 (91%)	87 (98%)	2 (2%)	45	29
1	I	84/98 (86%)	81 (96%)	3 (4%)	31	14
1	K	88/98 (90%)	86 (98%)	2 (2%)	44	27
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%)	17	5
2	J	27/33 (82%)	27 (100%)	0	100	100
2	L	29/33 (88%)	27 (93%)	2 (7%)	14	4
All	All	725/786 (92%)	707 (98%)	18 (2%)	42	24

All (18) 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	C	321	VAL
1	E	230	PHE
1	G	230	PHE
1	G	301	GLN
2	H	144	THR
2	H	151	VAL
1	I	229	VAL
1	I	245	THR
1	I	288	GLU
1	K	230	PHE
1	K	295	ILE
2	L	151	VAL
2	L	172	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	157	GLN
2	F	157	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	0.50	0	2,2,2	0.37	0
4	NHE	C	1	-	13,13,13	2.85	4 (30%)	16,17,17	1.15	2 (12%)
3	EDO	E	1	-	3,3,3	0.40	0	2,2,2	0.30	0
3	EDO	H	3	-	3,3,3	0.43	0	2,2,2	0.33	0
3	EDO	C	4	-	3,3,3	0.45	0	2,2,2	0.43	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	-	-	1/1/1/1	-
4	NHE	C	1	-	-	0/7/15/15	0/1/1/1
3	EDO	E	1	-	-	0/1/1/1	-
3	EDO	H	3	-	-	0/1/1/1	-
3	EDO	C	4	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NHE	O2-S	6.92	1.64	1.45
4	C	1	NHE	O1-S	4.83	1.58	1.45
4	C	1	NHE	O3-S	4.23	1.63	1.47
4	C	1	NHE	C2-S	2.56	1.81	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	NHE	C1-N-C1'	-2.52	109.34	114.18
4	C	1	NHE	O1-S-C2	2.49	110.49	106.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	EDO	O1-C1-C2-O2
3	C	4	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	EDO	4	0
3	C	4	EDO	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	111/111 (100%)	0.54	9 (8%)	18 19	13, 26, 44, 52	1 (0%)
1	C	111/111 (100%)	0.28	6 (5%)	31 34	14, 22, 56, 77	2 (1%)
1	E	101/111 (90%)	0.80	7 (6%)	23 25	22, 32, 56, 80	0
1	G	99/111 (89%)	0.94	15 (15%)	5 5	19, 34, 62, 67	1 (1%)
1	I	95/111 (85%)	1.11	14 (14%)	6 5	28, 38, 67, 82	0
1	K	100/111 (90%)	0.86	13 (13%)	7 7	17, 32, 64, 85	0
2	B	31/37 (83%)	0.04	1 (3%)	50 54	14, 20, 44, 50	0
2	D	34/37 (91%)	0.14	2 (5%)	28 31	16, 21, 41, 47	0
2	F	32/37 (86%)	1.00	2 (6%)	26 28	27, 41, 53, 55	0
2	H	36/37 (97%)	1.03	6 (16%)	4 4	26, 35, 57, 58	0
2	J	30/37 (81%)	1.12	1 (3%)	49 53	28, 42, 59, 60	0
2	L	32/37 (86%)	1.41	7 (21%)	2 2	25, 48, 68, 69	0
All	All	812/888 (91%)	0.75	83 (10%)	12 12	13, 32, 61, 85	4 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	ALA	6.7
1	C	243	ALA	5.5
1	E	272	LEU	5.3
1	E	285	THR	4.9
1	K	321	VAL	4.8
1	A	224	SER	4.4
2	H	144	THR	4.3
2	L	151	VAL	4.1
1	C	242	SER	4.0
1	I	272	LEU	3.7
1	G	321	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	286	ALA	3.5
1	G	273	ARG	3.5
1	K	274	SER	3.4
1	G	298	ALA	3.3
1	I	243	ALA	3.3
1	K	286	ALA	3.2
2	F	159	LEU	3.1
1	E	269	LEU	3.0
1	G	242	SER	3.0
1	E	286	ALA	3.0
1	G	272	LEU	2.9
2	H	166	VAL	2.9
1	G	297	THR	2.8
2	L	155	THR	2.8
2	L	156	ALA	2.8
2	H	179	SER	2.8
2	F	145	ARG	2.8
1	A	225	GLU	2.8
2	H	165	ASN	2.7
1	K	223	ALA	2.7
1	K	333	LYS	2.7
1	K	269	LEU	2.7
1	I	292	THR	2.7
2	D	144	THR	2.7
1	K	319	TRP	2.7
1	E	223	ALA	2.7
1	A	333	LYS	2.6
1	C	239	LYS	2.6
1	G	283	LEU	2.6
1	K	272	LEU	2.6
2	H	164	GLY	2.6
1	A	284	ASP	2.6
1	I	269	LEU	2.6
1	C	241	ASP	2.6
2	L	172	ASP	2.6
1	K	224	SER	2.6
1	K	271	GLU	2.6
1	E	283	LEU	2.5
1	G	274	SER	2.5
1	C	321	VAL	2.5
1	I	321	VAL	2.5
1	I	285	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	150	ASN	2.5
1	A	276	GLY	2.5
1	K	265	VAL	2.5
1	G	237	MET	2.5
1	A	297	THR	2.4
1	A	298	ALA	2.4
1	I	332	THR	2.4
1	C	333	LYS	2.4
2	J	150	ASN	2.4
1	I	267	LEU	2.4
2	L	154	SER	2.3
2	H	162	THR	2.3
1	G	224	SER	2.3
1	I	284	ASP	2.3
1	G	286	ALA	2.3
1	E	236	LEU	2.3
1	I	322	ASN	2.2
1	K	273	ARG	2.2
2	D	165	ASN	2.2
1	G	289	LYS	2.2
1	K	318	TYR	2.2
1	I	238	GLU	2.1
1	A	277	GLU	2.1
1	I	273	ARG	2.1
1	G	226	ILE	2.1
2	B	149	LYS	2.1
2	L	157	GLN	2.1
1	G	320	LYS	2.1
1	I	289	LYS	2.1
1	G	282	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	EDO	C	4	4/4	0.84	0.25	23,25,39,46	0
3	EDO	H	3	4/4	0.88	0.11	36,46,52,54	0
3	EDO	E	1	4/4	0.89	0.14	36,40,42,44	0
3	EDO	A	2	4/4	0.96	0.07	19,23,25,26	0
4	NHE	C	1	13/13	0.97	0.07	13,16,19,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.