



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:54 AM UTC

PDB ID : 8EI1 / pdb_00008ei1
Title : Crystal structure of the N-terminal domain of CUL4B in complex with H316, a Helicon Polypeptide
Authors : Li, K.; Tokareva, O.S.; Thomson, T.M.; Verdine, G.L.; McGee, J.H.
Deposited on : 2022-09-14
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 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:

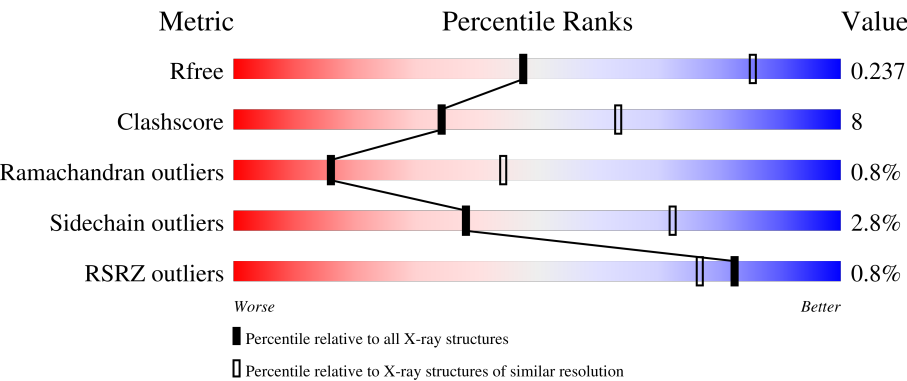
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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	354	80%16%..
1	B	354	% 77%20%..
1	C	354	% 76%18%.5%
1	D	354	% 71%22%.5%
2	E	19	79%21%

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Mol	Chain	Length	Quality of chain
2	F	19	84% 16%
2	G	19	5% 68% 11% 21%
2	H	19	11% 47% 16% 5% 32%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11809 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 Cullin-4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2843	1805	492	533	13			
1	B	344	Total	C	N	O	S	0	0	0
			2841	1804	492	532	13			
1	C	337	Total	C	N	O	S	0	0	0
			2778	1764	480	521	13			
1	D	338	Total	C	N	O	S	0	0	0
			2783	1767	480	523	13			

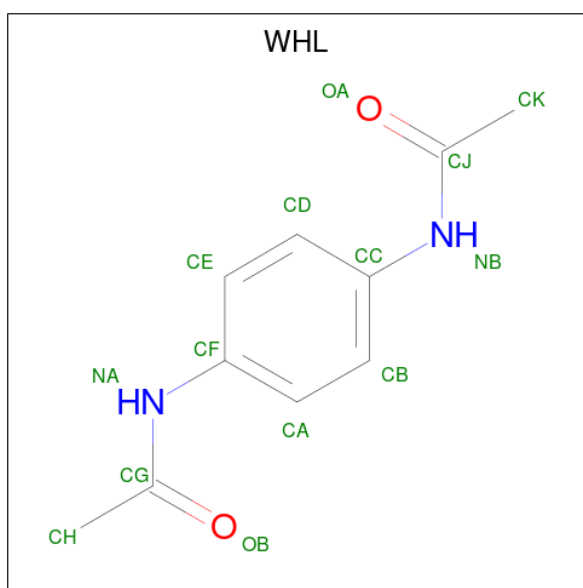
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	SER	-	expression tag	UNP Q13620
A	187	MET	-	expression tag	UNP Q13620
A	498	ARG	VAL	conflict	UNP Q13620
A	502	ASP	LEU	conflict	UNP Q13620
B	186	SER	-	expression tag	UNP Q13620
B	187	MET	-	expression tag	UNP Q13620
B	498	ARG	VAL	conflict	UNP Q13620
B	502	ASP	LEU	conflict	UNP Q13620
C	186	SER	-	expression tag	UNP Q13620
C	187	MET	-	expression tag	UNP Q13620
C	498	ARG	VAL	conflict	UNP Q13620
C	502	ASP	LEU	conflict	UNP Q13620
D	186	SER	-	expression tag	UNP Q13620
D	187	MET	-	expression tag	UNP Q13620
D	498	ARG	VAL	conflict	UNP Q13620
D	502	ASP	LEU	conflict	UNP Q13620

- Molecule 2 is a protein called H316.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	19	Total	C	N	O	S	0	0	1
			143	90	23	28	2			
2	F	19	Total	C	N	O	S	0	0	1
			143	90	23	28	2			
2	G	15	Total	C	N	O	S	0	0	0
			114	72	17	23	2			
2	H	13	Total	C	N	O	S	0	0	0
			108	67	18	21	2			

- Molecule 3 is N,N'-(1,4-phenylene)diacetamide (CCD ID: WHL) (formula: C₁₀H₁₂N₂O₂).

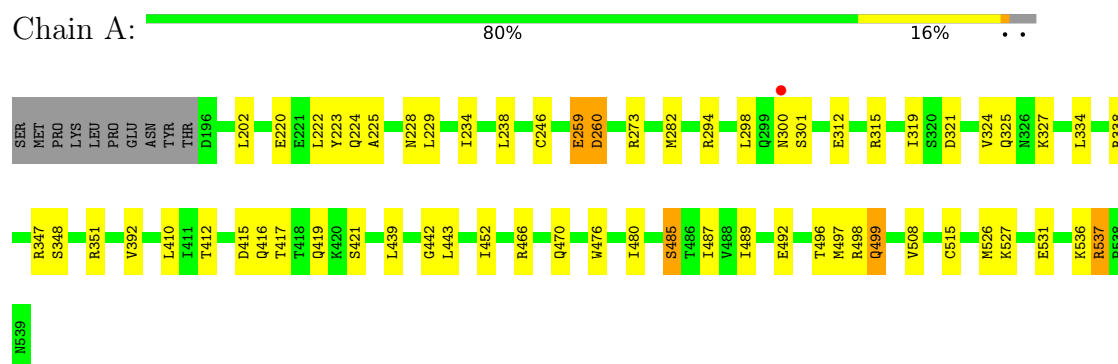


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			14	10	2	2		
3	F	1	Total	C	N	O	0	0
			14	10	2	2		
3	G	1	Total	C	N	O	0	0
			14	10	2	2		
3	H	1	Total	C	N	O	0	0
			14	10	2	2		

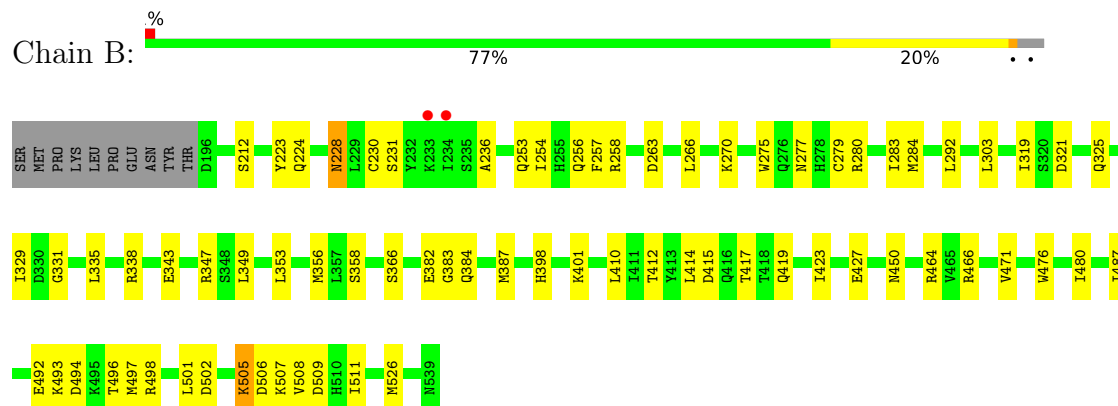
3 Residue-property plots

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.

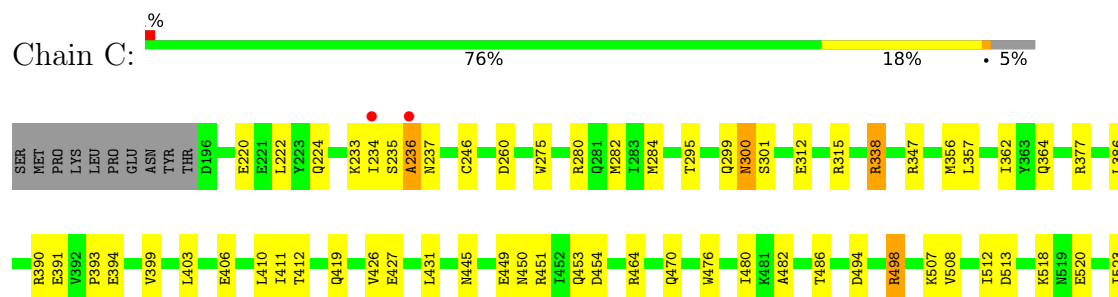
• Molecule 1: Cullin-4B

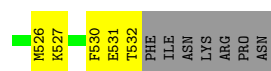


• Molecule 1: Cullin-4B

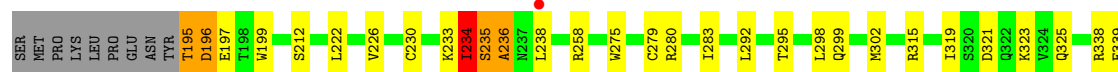


• Molecule 1: Cullin-4B

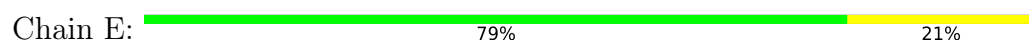




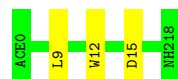
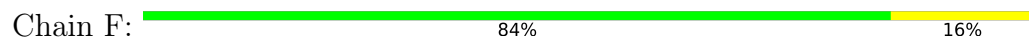
• Molecule 1: Cullin-4B



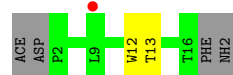
• Molecule 2: H316



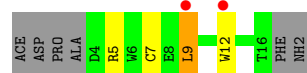
• Molecule 2: H316



• Molecule 2: H316



• Molecule 2: H316



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.65Å 99.65Å 366.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.82 – 2.89 49.82 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.82-2.89) 99.9 (49.82-2.89)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.212 , 0.254 (Not available) , 0.237	Depositor DCC
R_{free} test set	2102 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11809	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: WHL, NH2, ACE

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	0.23	0/2887	0.51	1/3890 (0.0%)
1	B	0.25	0/2885	0.51	0/3887
1	C	0.21	0/2820	0.48	0/3799
1	D	0.21	0/2825	0.55	2/3807 (0.1%)
2	E	0.21	0/145	0.44	0/200
2	F	0.18	0/145	0.34	0/200
2	G	0.17	0/118	0.45	0/163
2	H	0.25	0/111	0.59	0/152
All	All	0.23	0/11936	0.51	3/16098 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	SER	N-CA-C	-11.55	98.21	111.03
1	D	236	ALA	N-CA-C	5.47	122.45	110.80
1	A	260	ASP	N-CA-C	5.10	119.15	111.81

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	2843	0	2844	42	0
1	B	2841	0	2839	48	0
1	C	2778	0	2779	40	0
1	D	2783	0	2779	60	0
2	E	143	0	118	5	0
2	F	143	0	118	3	0
2	G	114	0	91	2	0
2	H	108	0	89	10	0
3	E	14	0	0	2	0
3	F	14	0	0	0	0
3	G	14	0	0	0	0
3	H	14	0	0	1	0
All	All	11809	0	11657	178	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 8.

All (178) 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:D:491:PRO:HB3	2:H:5:ARG:HH22	1.33	0.91
1:D:491:PRO:HG3	2:H:5:ARG:HH12	1.36	0.90
1:D:347:ARG:HD3	1:D:412:THR:HG21	1.52	0.89
1:B:410:LEU:HD21	1:B:419:GLN:HA	1.61	0.80
1:C:410:LEU:HD21	1:C:419:GLN:HA	1.67	0.74
2:H:9:LEU:HD22	2:H:9:LEU:O	1.87	0.74
1:D:497:MET:HG3	2:H:5:ARG:HH21	1.55	0.71
1:B:329:ILE:HD11	1:B:366:SER:HB3	1.72	0.71
1:D:387:MET:O	1:D:441:LYS:NZ	2.23	0.71
1:D:195:THR:OG1	1:D:196:ASP:N	2.20	0.71
1:A:347:ARG:HD3	1:A:412:THR:HG21	1.73	0.71
1:B:401:LYS:NZ	1:D:404:GLU:OE1	2.24	0.71
1:D:492:GLU:O	1:D:494:ASP:N	2.26	0.69
1:A:351:ARG:HD3	1:D:298:LEU:HD23	1.74	0.69
1:B:224:GLN:O	1:B:228:ASN:ND2	2.27	0.68
1:D:364:GLN:H	1:D:364:GLN:CD	2.02	0.66
1:C:531:GLU:HA	2:G:13:THR:HG21	1.78	0.65
1:C:312:GLU:OE1	1:C:315:ARG:NH1	2.29	0.65
1:B:347:ARG:HD3	1:B:412:THR:HG21	1.81	0.63
1:C:220:GLU:OE2	1:C:224:GLN:NE2	2.32	0.62
1:D:258:ARG:NH2	1:D:321:ASP:OD2	2.33	0.62
1:D:497:MET:HG3	2:H:5:ARG:NH2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:TRP:CH2	1:A:508:VAL:HG13	2.36	0.61
1:A:498:ARG:NH2	2:E:15:ASP:OD2	2.34	0.60
1:C:513:ASP:OD1	1:C:518:LYS:NZ	2.31	0.60
1:C:391:GLU:HB2	1:C:394:GLU:OE2	2.02	0.59
1:D:427:GLU:OE2	1:D:464:ARG:NH1	2.34	0.59
1:B:496:THR:O	1:B:498:ARG:N	2.34	0.59
1:B:498:ARG:NH2	2:F:15:ASP:OD2	2.36	0.58
1:A:298:LEU:HD13	1:D:348:SER:HB2	1.86	0.58
1:B:253:GLN:O	1:B:256:GLN:HG2	2.03	0.58
1:C:450:ASN:HB2	1:C:507:LYS:HE3	1.85	0.58
1:A:348:SER:HB3	1:D:298:LEU:HD13	1.86	0.58
1:C:235:SER:C	1:C:237:ASN:H	2.12	0.58
1:C:357:LEU:HD22	1:C:362:ILE:HD11	1.86	0.58
1:A:260:ASP:HB2	1:A:327:LYS:HD3	1.86	0.58
1:A:470:GLN:NE2	1:B:231:SER:O	2.36	0.57
1:C:338:ARG:CG	1:C:338:ARG:HH11	2.17	0.57
1:A:319:ILE:O	1:A:325:GLN:HB2	2.05	0.57
1:D:323:LYS:HD3	1:D:323:LYS:H	1.70	0.57
1:A:415:ASP:OD2	1:A:417:THR:HG23	2.04	0.56
1:C:233:LYS:HG2	1:C:234:ILE:H	1.70	0.56
1:B:228:ASN:HA	1:B:231:SER:HB2	1.88	0.56
1:B:349:LEU:O	1:B:353:LEU:HD12	2.05	0.56
1:D:439:LEU:HD12	1:D:443:LEU:HB2	1.88	0.56
1:B:258:ARG:NH2	1:B:321:ASP:OD2	2.34	0.56
1:A:224:GLN:NE2	1:A:228:ASN:OD1	2.38	0.56
1:D:199:TRP:CE3	1:D:238:LEU:HD11	2.39	0.56
1:D:302:MET:HE3	1:D:302:MET:HA	1.87	0.56
1:C:301:SER:OG	1:D:466:ARG:NH2	2.38	0.55
1:C:508:VAL:O	1:C:512:ILE:HD12	2.06	0.55
1:C:482:ALA:O	1:C:486:THR:HG23	2.07	0.54
2:H:9:LEU:HD22	2:H:9:LEU:C	2.31	0.54
1:D:393:PRO:HB3	1:D:454:ASP:OD2	2.08	0.54
1:C:445:ASN:O	1:C:449:GLU:HG2	2.08	0.54
1:D:275:TRP:CD2	1:D:356:MET:HG3	2.43	0.53
1:B:492:GLU:O	1:B:494:ASP:N	2.40	0.53
1:A:485:SER:O	1:A:489:ILE:HG13	2.08	0.53
1:C:520:GLU:HA	1:C:523:ILE:HD12	1.88	0.53
1:D:524:ASN:HA	1:D:527:LYS:HG2	1.91	0.53
1:B:480:ILE:HD13	1:B:526:MET:HG3	1.89	0.53
1:B:263:ASP:OD2	1:B:266:LEU:HD23	2.08	0.53
1:B:277:ASN:OD1	1:B:280:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:ALA:O	1:D:384:GLN:HG2	2.10	0.52
1:D:386:LEU:HD22	1:D:390:ARG:NE	2.24	0.52
1:B:257:PHE:CE1	1:B:270:LYS:HG2	2.44	0.52
1:A:476:TRP:HH2	1:A:508:VAL:HG13	1.72	0.51
1:B:427:GLU:OE2	1:B:464:ARG:NH1	2.44	0.51
1:A:496:THR:OG1	1:A:499:GLN:OE1	2.20	0.51
1:B:331:GLY:O	1:B:335:LEU:HG	2.11	0.51
1:A:202:LEU:HD23	1:A:222:LEU:HD22	1.92	0.51
1:A:351:ARG:HD3	1:D:298:LEU:CD2	2.41	0.51
1:B:257:PHE:HE1	1:B:270:LYS:HG2	1.75	0.51
2:E:1:ASP:OD1	2:E:2:PRO:HD3	2.11	0.51
1:A:223:TYR:CE2	1:D:280:ARG:HD2	2.46	0.50
1:A:537:ARG:NH1	3:E:101:WHL:OB	2.42	0.50
1:A:224:GLN:HE21	1:A:228:ASN:CG	2.20	0.50
1:D:315:ARG:NH2	1:D:360:LEU:O	2.45	0.50
1:C:406:GLU:HG3	1:C:426:VAL:HG21	1.94	0.50
1:D:445:ASN:C	1:D:445:ASN:HD22	2.19	0.50
1:D:222:LEU:O	1:D:226:VAL:HG23	2.12	0.49
1:B:476:TRP:CH2	1:B:508:VAL:HG13	2.47	0.49
2:E:1:ASP:HB2	2:E:5:ARG:NH2	2.28	0.49
1:B:492:GLU:C	1:B:494:ASP:H	2.21	0.49
1:A:527:LYS:HE2	1:A:531:GLU:OE2	2.13	0.49
1:B:410:LEU:HD21	1:B:419:GLN:HG2	1.95	0.49
1:A:410:LEU:HD11	1:A:419:GLN:HA	1.94	0.48
1:A:229:LEU:HB2	1:A:238:LEU:HD22	1.95	0.48
1:D:233:LYS:HE3	1:D:236:ALA:HB1	1.95	0.48
1:C:470:GLN:HE21	1:D:233:LYS:HG3	1.77	0.48
1:B:476:TRP:CZ2	1:B:508:VAL:HG13	2.49	0.48
1:D:195:THR:HG22	1:D:234:ILE:HD13	1.96	0.48
1:D:410:LEU:HA	1:D:414:LEU:HB2	1.95	0.48
1:D:230:CYS:SG	1:D:292:LEU:HD13	2.53	0.48
1:A:220:GLU:HB2	1:D:212:SER:HB3	1.95	0.47
1:A:439:LEU:HD22	1:A:443:LEU:HD22	1.96	0.47
1:B:275:TRP:CD2	1:B:356:MET:HG3	2.50	0.47
1:D:410:LEU:HD11	1:D:419:GLN:HA	1.97	0.47
1:A:298:LEU:HD22	1:D:351:ARG:HD3	1.96	0.47
1:A:334:LEU:O	1:A:338:ARG:HG3	2.14	0.47
1:B:338:ARG:HD3	1:B:343:GLU:OE1	2.13	0.47
2:H:7:CYS:HA	3:H:101:WHL:OB	2.14	0.47
2:E:5:ARG:HG2	2:E:5:ARG:HH11	1.79	0.47
1:C:427:GLU:OE2	1:C:464:ARG:NH1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:HG21	1:A:442:GLY:HA3	1.97	0.46
1:D:233:LYS:HE3	1:D:236:ALA:CB	2.44	0.46
1:D:491:PRO:CG	2:H:5:ARG:HH12	2.15	0.46
1:A:246:CYS:SG	1:A:282:MET:HE1	2.55	0.46
1:B:502:ASP:O	1:B:506:ASP:OD2	2.33	0.46
1:B:223:TYR:CE2	1:C:280:ARG:HD2	2.51	0.46
1:C:476:TRP:CH2	1:C:508:VAL:HG13	2.51	0.46
1:C:347:ARG:HD3	1:C:412:THR:HG21	1.98	0.46
1:C:393:PRO:HB3	1:C:454:ASP:OD2	2.15	0.46
1:B:505:LYS:HE3	1:B:509:ASP:OD2	2.16	0.46
1:D:442:GLY:O	1:D:446:LEU:HD13	2.16	0.45
1:B:415:ASP:OD2	1:B:417:THR:HG23	2.17	0.45
1:C:338:ARG:CG	1:C:338:ARG:NH1	2.75	0.45
1:D:508:VAL:O	1:D:512:ILE:HD12	2.16	0.45
1:C:246:CYS:SG	1:C:282:MET:HE1	2.56	0.45
1:B:212:SER:HB3	1:C:220:GLU:HB2	1.98	0.45
1:C:220:GLU:O	1:C:224:GLN:HG2	2.17	0.45
1:A:312:GLU:CD	1:A:315:ARG:HH12	2.23	0.44
1:A:537:ARG:HH12	3:E:101:WHL:CG	2.30	0.44
1:B:254:ILE:HD11	1:B:321:ASP:OD2	2.18	0.44
1:C:526:MET:HE2	1:C:526:MET:HB3	1.89	0.44
1:D:527:LYS:HG3	1:D:528:GLU:N	2.32	0.44
1:A:466:ARG:CZ	1:B:236:ALA:HB2	2.48	0.44
1:D:279:CYS:O	1:D:283:ILE:HG13	2.18	0.44
1:D:468:GLY:O	1:D:471:VAL:HG12	2.18	0.44
1:D:275:TRP:CE2	1:D:356:MET:HG3	2.53	0.43
1:D:319:ILE:O	1:D:325:GLN:HB2	2.18	0.43
1:C:480:ILE:HD13	1:C:526:MET:HG3	1.99	0.43
2:E:1:ASP:CG	2:E:2:PRO:HD3	2.43	0.43
1:A:301:SER:HA	1:B:466:ARG:NH1	2.32	0.43
1:C:234:ILE:HG22	1:C:236:ALA:H	1.82	0.43
1:A:225:ALA:O	1:A:229:LEU:HG	2.19	0.43
1:B:410:LEU:HA	1:B:414:LEU:HB2	2.00	0.43
1:D:323:LYS:HD3	1:D:323:LYS:N	2.32	0.43
1:A:419:GLN:NE2	1:C:411:ILE:HG23	2.34	0.43
1:C:403:LEU:HD13	1:C:464:ARG:CZ	2.49	0.43
1:D:295:THR:O	1:D:299:GLN:N	2.44	0.43
1:A:321:ASP:HB3	1:A:324:VAL:HB	2.00	0.42
1:A:480:ILE:HD13	1:A:526:MET:HG3	2.01	0.42
1:A:294:ARG:O	1:A:298:LEU:HG	2.19	0.42
1:B:410:LEU:CD2	1:B:419:GLN:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:CYS:SG	1:B:292:LEU:HD13	2.60	0.42
1:C:299:GLN:O	1:C:300:ASN:CB	2.67	0.42
1:C:399:VAL:HG11	1:C:431:LEU:HD21	2.00	0.42
1:D:435:LEU:O	1:D:439:LEU:HD22	2.19	0.42
1:D:501:LEU:HD22	2:H:12:TRP:CE2	2.54	0.42
1:B:501:LEU:HD11	2:F:9:LEU:HD12	2.00	0.42
1:B:383:GLY:O	1:B:387:MET:HB2	2.20	0.42
1:A:487:ILE:HG23	1:A:497:MET:HE3	2.01	0.42
1:B:382:GLU:OE2	1:B:398:HIS:NE2	2.50	0.42
1:A:300:ASN:HD21	1:B:423:ILE:HB	1.84	0.41
1:D:238:LEU:HA	1:D:238:LEU:HD12	1.77	0.41
1:B:319:ILE:O	1:B:325:GLN:HB2	2.20	0.41
1:C:386:LEU:HD22	1:C:390:ARG:NE	2.35	0.41
1:D:498:ARG:HH11	2:H:12:TRP:HD1	1.68	0.41
1:A:470:GLN:NE2	1:B:231:SER:C	2.78	0.41
1:D:447:LEU:HD13	1:D:479:TYR:CD2	2.56	0.41
1:A:452:ILE:HG23	1:A:515:CYS:SG	2.60	0.41
1:B:507:LYS:O	1:B:511:ILE:HG13	2.20	0.41
1:C:235:SER:C	1:C:237:ASN:N	2.76	0.41
1:B:498:ARG:NE	2:F:12:TRP:HD1	2.18	0.41
1:D:446:LEU:HB3	1:D:455:LEU:HD21	2.03	0.41
1:B:279:CYS:O	1:B:283:ILE:HG13	2.21	0.41
1:B:487:ILE:HD12	1:B:487:ILE:HA	1.90	0.41
1:D:379:TYR:OH	1:D:406:GLU:OE2	2.30	0.41
1:C:275:TRP:CD2	1:C:356:MET:HG3	2.56	0.41
1:D:482:ALA:O	1:D:486:THR:HG23	2.21	0.41
1:A:259:GLU:O	1:A:259:GLU:CG	2.69	0.41
1:D:338:ARG:HD3	1:D:343:GLU:OE1	2.21	0.40
1:D:339:GLU:HG2	1:D:409:ARG:HH21	1.87	0.40
1:D:407:ALA:O	1:D:411:ILE:HG12	2.21	0.40
1:B:284:MET:HG3	1:C:284:MET:HG3	2.03	0.40
1:C:498:ARG:HE	1:C:498:ARG:HB3	1.75	0.40
1:C:530:PHE:CG	2:G:12:TRP:HZ3	2.39	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	342/354 (97%)	330 (96%)	10 (3%)	2 (1%)	21	51
1	B	342/354 (97%)	330 (96%)	10 (3%)	2 (1%)	21	51
1	C	335/354 (95%)	323 (96%)	8 (2%)	4 (1%)	10	34
1	D	336/354 (95%)	320 (95%)	12 (4%)	4 (1%)	10	34
2	E	17/19 (90%)	16 (94%)	1 (6%)	0	100	100
2	F	17/19 (90%)	16 (94%)	1 (6%)	0	100	100
2	G	13/19 (68%)	13 (100%)	0	0	100	100
2	H	11/19 (58%)	10 (91%)	1 (9%)	0	100	100
All	All	1413/1492 (95%)	1358 (96%)	43 (3%)	12 (1%)	16	44

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	492	GLU
1	B	493	LYS
1	B	497	MET
1	D	493	LYS
1	A	234	ILE
1	C	236	ALA
1	C	260	ASP
1	C	300	ASN
1	C	494	ASP
1	D	196	ASP
1	D	234	ILE
1	D	197	GLU

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	313/330 (95%)	305 (97%)	8 (3%)	40	73
1	B	312/330 (94%)	305 (98%)	7 (2%)	45	77
1	C	305/330 (92%)	295 (97%)	10 (3%)	33	67
1	D	305/330 (92%)	295 (97%)	10 (3%)	33	67
2	E	14/14 (100%)	14 (100%)	0	100	100
2	F	14/14 (100%)	14 (100%)	0	100	100
2	G	11/14 (79%)	11 (100%)	0	100	100
2	H	11/14 (79%)	10 (91%)	1 (9%)	9	28
All	All	1285/1376 (93%)	1249 (97%)	36 (3%)	38	72

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	GLU
1	A	273	ARG
1	A	416	GLN
1	A	421	SER
1	A	485	SER
1	A	499	GLN
1	A	536	LYS
1	A	537	ARG
1	B	228	ASN
1	B	303	LEU
1	B	358	SER
1	B	384	GLN
1	B	450	ASN
1	B	471	VAL
1	B	505	LYS
1	C	222	LEU
1	C	295	THR
1	C	338	ARG
1	C	364	GLN
1	C	377	ARG
1	C	451	ARG
1	C	453	GLN
1	C	498	ARG

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Mol	Chain	Res	Type
1	C	527	LYS
1	C	532	THR
1	D	195	THR
1	D	234	ILE
1	D	235	SER
1	D	362	ILE
1	D	364	GLN
1	D	378	LEU
1	D	421	SER
1	D	439	LEU
1	D	445	ASN
1	D	532	THR
2	H	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
1	A	322	GLN
1	A	434	HIS
1	B	322	GLN
1	B	325	GLN
1	C	249	HIS
1	C	281	GLN
1	C	434	HIS
1	D	325	GLN
1	D	434	HIS
1	D	445	ASN
1	D	450	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	WHL	E	101	2	14,14,14	2.38	5 (35%)	18,18,18	1.10	1 (5%)
3	WHL	H	101	2	14,14,14	2.79	4 (28%)	18,18,18	1.20	3 (16%)
3	WHL	F	101	2	14,14,14	2.41	4 (28%)	18,18,18	1.16	2 (11%)
3	WHL	G	101	2	14,14,14	2.76	5 (35%)	18,18,18	1.88	4 (22%)

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	WHL	E	101	2	-	0/8/8/8	0/1/1/1
3	WHL	H	101	2	-	0/8/8/8	0/1/1/1
3	WHL	F	101	2	-	0/8/8/8	0/1/1/1
3	WHL	G	101	2	-	0/8/8/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	101	WHL	CG-NA	6.60	1.48	1.36
3	G	101	WHL	CJ-NB	6.44	1.48	1.36
3	H	101	WHL	CJ-NB	5.74	1.46	1.36
3	F	101	WHL	CG-NA	5.60	1.46	1.36
3	G	101	WHL	CG-NA	5.56	1.46	1.36
3	E	101	WHL	CG-NA	5.37	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	101	WHL	CJ-NB	5.22	1.45	1.36
3	F	101	WHL	CJ-NB	5.06	1.45	1.36
3	G	101	WHL	CC-NB	3.59	1.48	1.41
3	H	101	WHL	CC-NB	2.88	1.47	1.41
3	H	101	WHL	CF-NA	2.83	1.47	1.41
3	F	101	WHL	CF-NA	2.49	1.46	1.41
3	E	101	WHL	CC-NB	2.43	1.46	1.41
3	E	101	WHL	CF-NA	2.40	1.46	1.41
3	G	101	WHL	CF-NA	2.36	1.46	1.41
3	F	101	WHL	CC-NB	2.32	1.46	1.41
3	G	101	WHL	OA-CJ	-2.24	1.18	1.23
3	E	101	WHL	OB-CG	-2.02	1.18	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	101	WHL	CK-CJ-NB	5.96	123.92	114.95
3	G	101	WHL	OA-CJ-CK	-3.39	116.02	122.05
3	E	101	WHL	CH-CG-NA	2.46	118.65	114.95
3	H	101	WHL	CH-CG-NA	2.41	118.58	114.95
3	F	101	WHL	CH-CG-NA	2.28	118.38	114.95
3	G	101	WHL	CC-NB-CJ	-2.24	123.80	127.98
3	G	101	WHL	OA-CJ-NB	-2.19	120.06	123.06
3	H	101	WHL	OB-CG-CH	-2.16	118.21	122.05
3	F	101	WHL	CK-CJ-NB	2.07	118.07	114.95
3	H	101	WHL	CE-CF-NA	2.01	127.15	120.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	101	WHL	2	0
3	H	101	WHL	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	344/354 (97%)	-0.49	1 (0%) 90 87	57, 73, 110, 135	0
1	B	344/354 (97%)	-0.31	2 (0%) 85 81	71, 92, 129, 157	0
1	C	337/354 (95%)	-0.31	2 (0%) 85 81	51, 85, 146, 168	0
1	D	338/354 (95%)	-0.34	3 (0%) 81 75	57, 82, 150, 187	0
2	E	17/19 (89%)	-0.38	0 100 100	59, 69, 97, 112	0
2	F	17/19 (89%)	-0.14	0 100 100	82, 94, 124, 136	0
2	G	15/19 (78%)	0.98	1 (6%) 24 19	133, 150, 168, 177	0
2	H	13/19 (68%)	0.92	2 (15%) 5 4	178, 188, 196, 201	0
All	All	1425/1492 (95%)	-0.34	11 (0%) 82 77	51, 84, 145, 201	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	236	ALA	4.5
1	D	532	THR	3.1
2	H	9	LEU	2.7
2	G	9	LEU	2.6
1	B	233	LYS	2.5
1	B	234	ILE	2.3
1	A	300	ASN	2.3
1	D	496	THR	2.2
1	D	238	LEU	2.2
1	C	234	ILE	2.2
2	H	12	TRP	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	WHL	H	101	14/14	0.13	0.13	189,191,193,193	0
3	WHL	G	101	14/14	0.27	0.11	150,152,153,153	0
3	WHL	F	101	14/14	0.85	0.12	78,95,116,116	0
3	WHL	E	101	14/14	0.90	0.10	54,69,90,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.