



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:30 PM UTC

PDB ID : 8G66 / pdb_00008g66
Title : Structure with SJ3149
Authors : Miller, D.J.; Young, S.M.; Fischer, M.
Deposited on : 2023-02-14
Resolution : 3.45 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

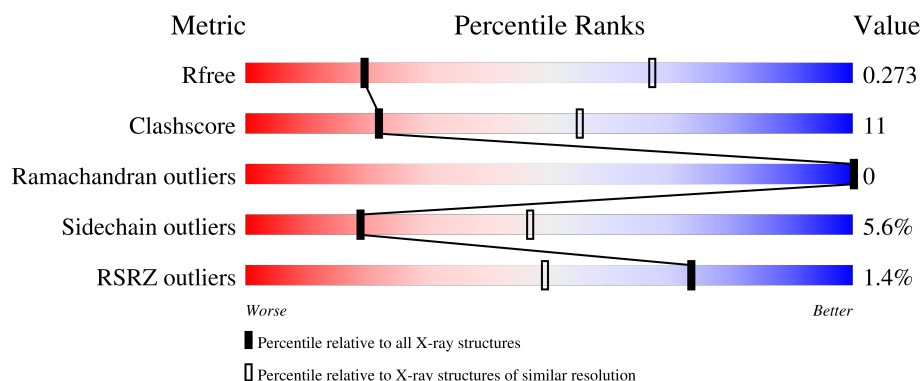
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	860	
1	D	860	
2	B	426	
2	E	426	
3	C	341	

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Mol	Chain	Length	Quality of chain
3	F	341	% 60%24%14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21297 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	778	Total	C	N	O	S	0	0	0
			5713	3630	954	1099	30			
1	D	779	Total	C	N	O	S	0	0	0
			5835	3714	971	1116	34			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP Q16531
A	-22	GLY	-	expression tag	UNP Q16531
A	-21	SER	-	expression tag	UNP Q16531
A	-20	SER	-	expression tag	UNP Q16531
A	-19	HIS	-	expression tag	UNP Q16531
A	-18	HIS	-	expression tag	UNP Q16531
A	-17	HIS	-	expression tag	UNP Q16531
A	-16	HIS	-	expression tag	UNP Q16531
A	-15	HIS	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	SER	-	expression tag	UNP Q16531
A	-12	ALA	-	expression tag	UNP Q16531
A	-11	VAL	-	expression tag	UNP Q16531
A	-10	ASP	-	expression tag	UNP Q16531
A	-9	GLU	-	expression tag	UNP Q16531
A	-8	ASN	-	expression tag	UNP Q16531
A	-7	LEU	-	expression tag	UNP Q16531
A	-6	TYR	-	expression tag	UNP Q16531
A	-5	PHE	-	expression tag	UNP Q16531
A	-4	GLN	-	expression tag	UNP Q16531
A	-3	GLY	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
A	700	GLY	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531
D	-23	MET	-	initiating methionine	UNP Q16531
D	-22	GLY	-	expression tag	UNP Q16531
D	-21	SER	-	expression tag	UNP Q16531
D	-20	SER	-	expression tag	UNP Q16531
D	-19	HIS	-	expression tag	UNP Q16531
D	-18	HIS	-	expression tag	UNP Q16531
D	-17	HIS	-	expression tag	UNP Q16531
D	-16	HIS	-	expression tag	UNP Q16531
D	-15	HIS	-	expression tag	UNP Q16531
D	-14	HIS	-	expression tag	UNP Q16531
D	-13	SER	-	expression tag	UNP Q16531
D	-12	ALA	-	expression tag	UNP Q16531
D	-11	VAL	-	expression tag	UNP Q16531
D	-10	ASP	-	expression tag	UNP Q16531
D	-9	GLU	-	expression tag	UNP Q16531
D	-8	ASN	-	expression tag	UNP Q16531
D	-7	LEU	-	expression tag	UNP Q16531
D	-6	TYR	-	expression tag	UNP Q16531
D	-5	PHE	-	expression tag	UNP Q16531
D	-4	GLN	-	expression tag	UNP Q16531
D	-3	GLY	-	expression tag	UNP Q16531
D	-2	GLY	-	expression tag	UNP Q16531
D	-1	GLY	-	expression tag	UNP Q16531
D	0	ARG	-	expression tag	UNP Q16531
D	700	GLY	-	linker	UNP Q16531
D	701	ASN	-	linker	UNP Q16531
D	702	GLY	-	linker	UNP Q16531
D	703	ASN	-	linker	UNP Q16531
D	704	SER	-	linker	UNP Q16531
D	705	GLY	-	linker	UNP Q16531

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	372	Total	C	N	O	S	0	0	0
			2841	1818	478	523	22			
2	E	303	Total	C	N	O	S	0	0	0
			2186	1399	371	398	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	MET	-	initiating methionine	UNP Q96SW2
B	18	ASP	-	expression tag	UNP Q96SW2
B	19	TRP	-	expression tag	UNP Q96SW2
B	20	SER	-	expression tag	UNP Q96SW2
B	21	HIS	-	expression tag	UNP Q96SW2
B	22	PRO	-	expression tag	UNP Q96SW2
B	23	GLN	-	expression tag	UNP Q96SW2
B	24	PHE	-	expression tag	UNP Q96SW2
B	25	GLU	-	expression tag	UNP Q96SW2
B	26	LYS	-	expression tag	UNP Q96SW2
B	27	SER	-	expression tag	UNP Q96SW2
B	28	ALA	-	expression tag	UNP Q96SW2
B	29	VAL	-	expression tag	UNP Q96SW2
B	30	ASP	-	expression tag	UNP Q96SW2
B	31	GLU	-	expression tag	UNP Q96SW2
B	32	ASN	-	expression tag	UNP Q96SW2
B	33	LEU	-	expression tag	UNP Q96SW2
B	34	TYR	-	expression tag	UNP Q96SW2
B	35	PHE	-	expression tag	UNP Q96SW2
B	36	GLN	-	expression tag	UNP Q96SW2
B	37	GLY	-	expression tag	UNP Q96SW2
B	38	GLY	-	expression tag	UNP Q96SW2
B	39	GLY	-	expression tag	UNP Q96SW2
B	40	ARG	-	expression tag	UNP Q96SW2
E	17	MET	-	initiating methionine	UNP Q96SW2
E	18	ASP	-	expression tag	UNP Q96SW2
E	19	TRP	-	expression tag	UNP Q96SW2
E	20	SER	-	expression tag	UNP Q96SW2
E	21	HIS	-	expression tag	UNP Q96SW2
E	22	PRO	-	expression tag	UNP Q96SW2
E	23	GLN	-	expression tag	UNP Q96SW2
E	24	PHE	-	expression tag	UNP Q96SW2
E	25	GLU	-	expression tag	UNP Q96SW2
E	26	LYS	-	expression tag	UNP Q96SW2
E	27	SER	-	expression tag	UNP Q96SW2
E	28	ALA	-	expression tag	UNP Q96SW2
E	29	VAL	-	expression tag	UNP Q96SW2
E	30	ASP	-	expression tag	UNP Q96SW2
E	31	GLU	-	expression tag	UNP Q96SW2
E	32	ASN	-	expression tag	UNP Q96SW2
E	33	LEU	-	expression tag	UNP Q96SW2
E	34	TYR	-	expression tag	UNP Q96SW2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	35	PHE	-	expression tag	UNP Q96SW2
E	36	GLN	-	expression tag	UNP Q96SW2
E	37	GLY	-	expression tag	UNP Q96SW2
E	38	GLY	-	expression tag	UNP Q96SW2
E	39	GLY	-	expression tag	UNP Q96SW2
E	40	ARG	-	expression tag	UNP Q96SW2

- Molecule 3 is a protein called Casein kinase I isoform alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	289	Total	C	N	O	S	0	0	0
			2311	1487	397	412	15			
3	F	294	Total	C	N	O	S	0	0	0
			2381	1534	412	421	14			

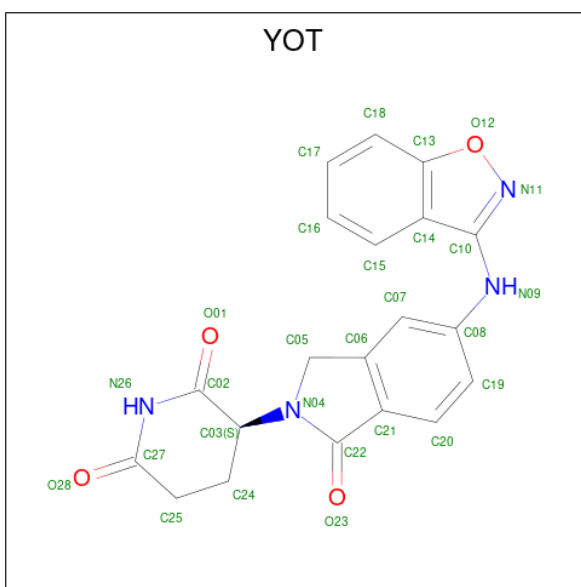
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P48729
C	-2	GLY	-	expression tag	UNP P48729
C	-1	GLY	-	expression tag	UNP P48729
C	0	ARG	-	expression tag	UNP P48729
F	-3	GLY	-	expression tag	UNP P48729
F	-2	GLY	-	expression tag	UNP P48729
F	-1	GLY	-	expression tag	UNP P48729
F	0	ARG	-	expression tag	UNP P48729

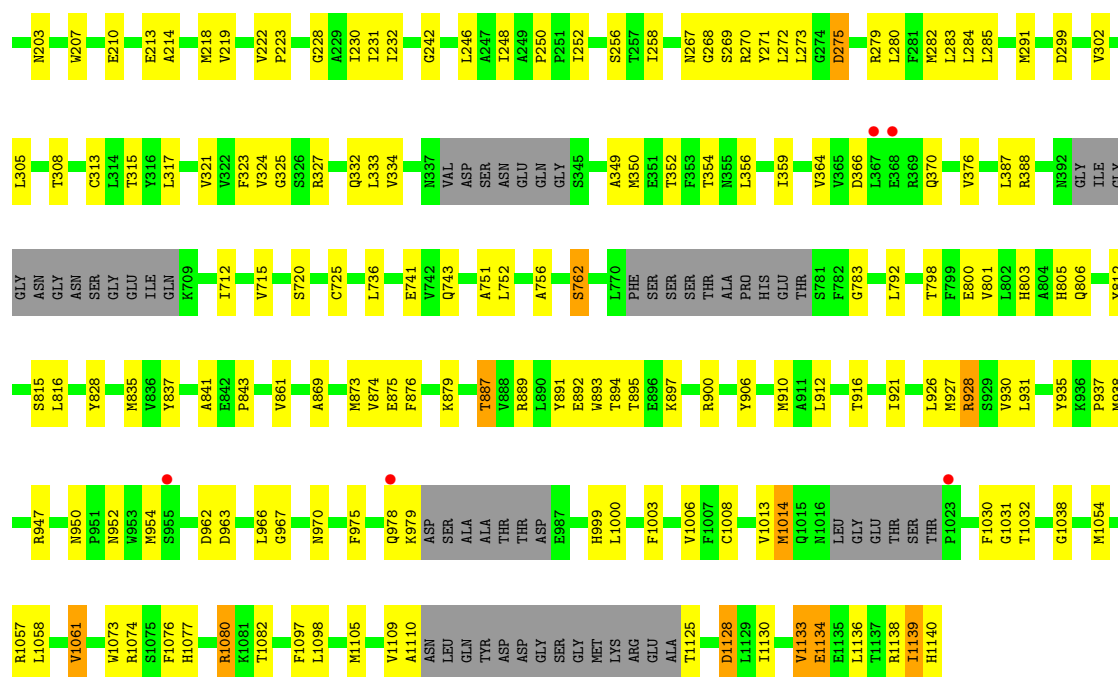
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		

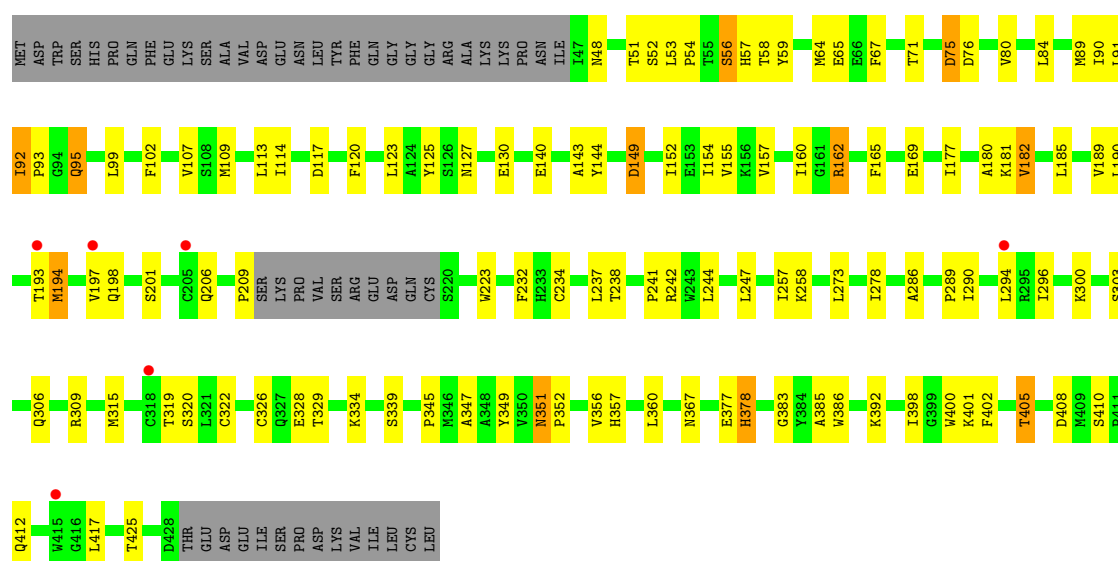
- Molecule 5 is (3S)-3-{5-[(1,2-benzoxazol-3-yl)amino]-1-oxo-1,3-dihydro-2H-isoindol-2-yl}piperidine-2,6-dione (CCD ID: YOT) (formula: C₂₀H₁₆N₄O₄) (labeled as "Ligand of Interest" by depositor).



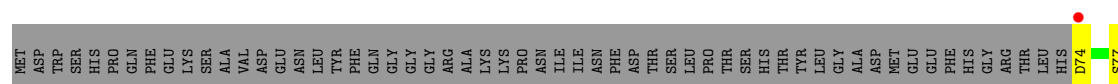
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			28	20	4	4		

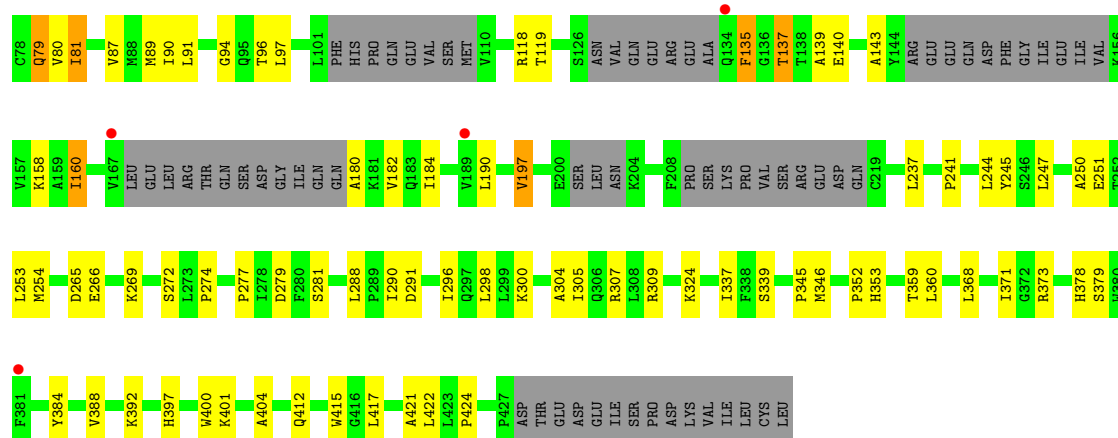


• Molecule 2: Protein cereblon

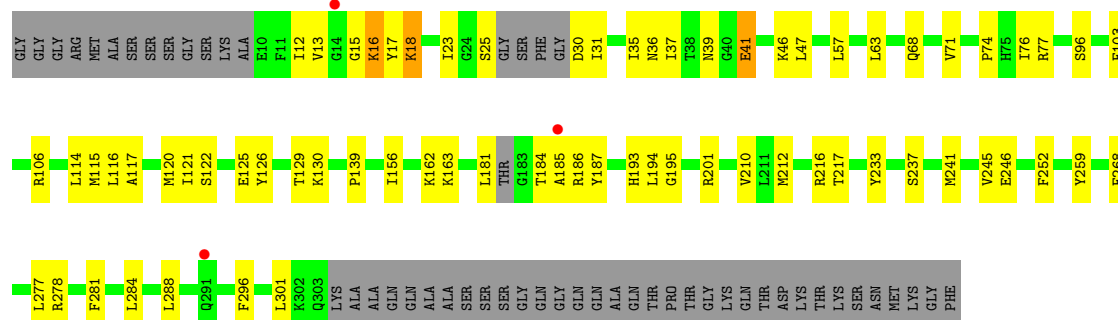


• Molecule 2: Protein cereblon

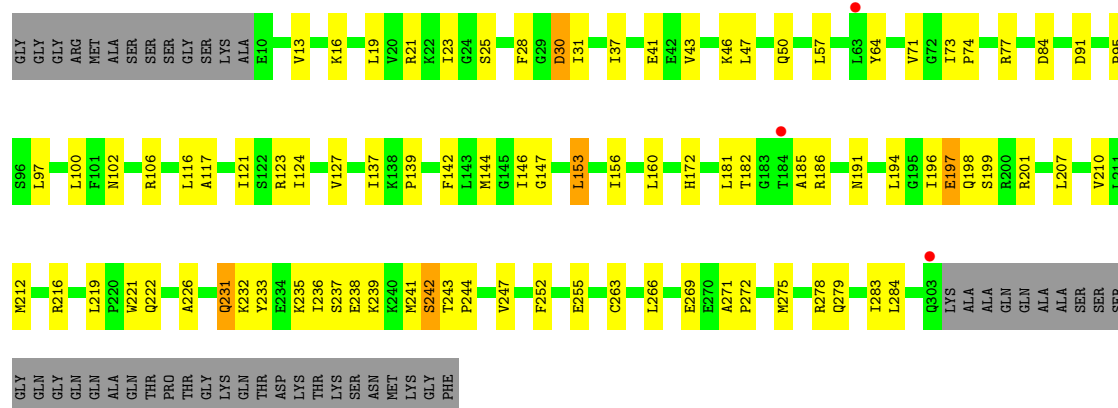




• Molecule 3: Casein kinase I isoform alpha



• Molecule 3: Casein kinase I isoform alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.66Å 109.71Å 112.34Å 105.49° 94.41° 100.03°	Depositor
Resolution (Å)	48.25 – 3.45 48.25 – 3.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.25-3.45) 97.1 (48.25-3.45)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.213 , 0.272 0.213 , 0.273	Depositor DCC
R_{free} test set	1999 reflections (3.85%)	wwPDB-VP
Wilson B-factor (Å ²)	106.9	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 81.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21297	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: YOT, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/5814	0.55	0/7920
1	D	0.42	0/5941	0.59	0/8076
2	B	0.43	0/2912	0.62	1/3979 (0.0%)
2	E	0.40	0/2238	0.56	0/3070
3	C	0.42	0/2364	0.58	0/3195
3	F	0.49	0/2438	0.62	0/3290
All	All	0.42	0/21707	0.58	1/29530 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	206	GLN	N-CA-C	5.74	118.02	111.02

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	5713	0	5335	105	0
1	D	5835	0	5541	135	0
2	B	2841	0	2669	73	0
2	E	2186	0	1932	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2311	0	2206	40	0
3	F	2381	0	2324	60	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	B	28	0	0	1	0
All	All	21297	0	20007	443	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 11.

All (443) 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)
3:F:16:LYS:HA	3:F:37:ILE:HG12	1.62	0.82
1:A:118:THR:HG21	1:A:165:ILE:HA	1.61	0.81
1:D:248:ILE:HG13	1:D:250:PRO:HD3	1.63	0.79
2:E:352:PRO:HG3	2:E:378:HIS:CD2	2.17	0.79
1:D:118:THR:HB	1:D:134:ARG:HH22	1.49	0.76
2:B:398:ILE:HG22	2:B:417:LEU:HD22	1.68	0.75
3:F:43:VAL:HG12	3:F:77:ARG:HH11	1.51	0.75
1:D:743:GLN:HB3	1:D:783:GLY:H	1.54	0.72
2:B:92:ILE:HD13	2:B:286:ALA:HA	1.70	0.71
3:F:19:LEU:HD21	3:F:47:LEU:HD11	1.72	0.71
1:A:252:ILE:HG22	1:A:281:PHE:HE2	1.55	0.71
1:D:916:THR:HG22	1:D:921:ILE:HG13	1.73	0.71
1:D:272:LEU:HD22	1:D:280:LEU:HD11	1.74	0.70
1:D:250:PRO:HG3	1:D:302:VAL:HG21	1.74	0.69
2:B:189:VAL:HG22	2:B:278:ILE:HD11	1.74	0.68
3:C:13:VAL:HG23	3:C:17:TYR:HB2	1.76	0.68
2:E:269:LYS:HA	2:E:272:SER:HB2	1.75	0.68
1:D:69:PRO:HD2	1:D:72:GLU:HG3	1.76	0.67
1:D:912:LEU:HD21	2:E:244:LEU:HD21	1.77	0.66
3:F:64:TYR:HE1	3:F:74:PRO:HD2	1.61	0.66
2:B:385:ALA:O	2:B:402:PHE:HA	1.96	0.65
1:D:1058:LEU:HD21	1:D:1097:PHE:HD1	1.62	0.65
3:F:16:LYS:O	3:F:37:ILE:N	2.29	0.65
2:E:290:ILE:HA	2:E:424:PRO:HG3	1.79	0.64
3:C:116:LEU:HB3	3:C:120:MET:HE2	1.79	0.64
1:D:230:ILE:HD11	1:D:285:LEU:HD21	1.79	0.64
3:F:185:ALA:HB2	3:F:233:TYR:CE1	2.33	0.64
3:F:275:MET:HE2	3:F:278:ARG:HH21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:SER:HB2	1:A:911:ALA:HB3	1.80	0.63
2:E:417:LEU:HB2	2:E:422:LEU:HD11	1.78	0.63
3:F:219:LEU:HD13	3:F:221:TRP:HE1	1.62	0.63
1:D:954:MET:HE3	1:D:975:PHE:HZ	1.63	0.63
3:C:117:ALA:O	3:C:121:ILE:HG13	1.99	0.62
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.82	0.62
1:D:43:VAL:HG23	1:D:52:VAL:HG21	1.82	0.62
2:B:351:ASN:ND2	3:C:37:ILE:O	2.29	0.62
1:A:207:TRP:CB	1:A:242:GLY:HA2	2.30	0.62
2:B:320:SER:HB3	2:B:425:THR:HB	1.83	0.61
2:E:90:ILE:HD13	2:E:296:ILE:HG13	1.83	0.61
1:D:58:TYR:HB3	1:D:1073:TRP:HB2	1.83	0.61
3:F:221:TRP:HB2	3:F:236:ILE:HG23	1.84	0.60
1:D:207:TRP:CB	1:D:242:GLY:HA2	2.31	0.60
2:E:143:ALA:HB3	2:E:158:LYS:H	1.66	0.60
1:D:356:LEU:HD21	1:D:712:ILE:HD13	1.82	0.59
2:B:194:MET:SD	2:B:232:PHE:HA	2.41	0.59
3:F:237:SER:O	3:F:241:MET:HG3	2.02	0.59
2:E:197:VAL:HG12	2:E:237:LEU:HD12	1.83	0.59
2:B:67:PHE:HZ	2:B:114:ILE:HG23	1.66	0.59
1:D:1013:VAL:HG11	1:D:1138:ARG:O	2.02	0.59
1:A:329:GLY:O	1:A:355:ASN:ND2	2.29	0.59
2:B:56:SER:HB2	2:B:58:THR:HG23	1.85	0.58
1:A:358:PRO:HD2	1:A:380:GLY:HA2	1.85	0.58
1:D:213:GLU:HG2	1:D:214:ALA:N	2.18	0.58
1:D:843:PRO:HG2	1:D:869:ALA:HB2	1.86	0.58
1:D:118:THR:HG21	1:D:165:ILE:O	2.03	0.58
3:C:114:LEU:HD22	3:C:281:PHE:HB3	1.86	0.58
1:A:912:LEU:HD21	2:B:244:LEU:HD11	1.86	0.58
3:F:244:PRO:HD2	3:F:247:VAL:HG21	1.86	0.57
1:A:196:SER:CB	1:A:199:GLU:HB2	2.35	0.57
2:B:80:VAL:HA	2:B:180:ALA:O	2.04	0.57
2:B:386:TRP:HA	2:B:401:LYS:O	2.04	0.57
1:D:928:ARG:HD2	1:D:950:ASN:O	2.04	0.57
2:B:289:PRO:HB3	2:B:360:LEU:HD22	1.84	0.57
1:D:1098:LEU:HD11	1:D:1133:VAL:HB	1.87	0.57
3:F:139:PRO:HG3	3:F:210:VAL:HG13	1.87	0.57
1:A:954:MET:HE3	1:A:975:PHE:HZ	1.69	0.57
1:A:124:ILE:HG12	1:A:131:ILE:HG12	1.86	0.56
3:C:139:PRO:HG3	3:C:210:VAL:HG13	1.87	0.56
2:E:404:ALA:HB2	2:E:412:GLN:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:194:LEU:HD21	3:F:241:MET:SD	2.44	0.56
3:C:12:ILE:HG13	3:C:18:LYS:HG2	1.86	0.56
1:D:223:PRO:HD2	1:D:268:GLY:HA3	1.86	0.56
3:F:226:ALA:HB3	3:F:231:GLN:HB3	1.86	0.56
1:A:261:HIS:HA	1:A:272:LEU:O	2.06	0.55
3:C:36:ASN:HB3	3:C:39:ASN:OD1	2.06	0.55
1:D:828:TYR:CE1	1:D:861:VAL:HG21	2.40	0.55
1:D:1130:ILE:O	1:D:1134:GLU:HG2	2.06	0.55
1:D:954:MET:HE3	1:D:975:PHE:CZ	2.40	0.55
1:D:910:MET:O	1:D:912:LEU:N	2.38	0.55
2:E:251:GLU:HA	2:E:254:MET:HE3	1.89	0.55
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.87	0.55
1:A:891:TYR:HB3	1:A:899:LEU:HD22	1.89	0.55
3:F:28:PHE:CZ	3:F:46:LYS:HG2	2.42	0.55
3:C:186:ARG:HD2	3:C:187:TYR:CZ	2.42	0.54
2:E:359:THR:HA	2:E:417:LEU:O	2.07	0.54
1:A:853:TYR:OH	1:A:856:GLY:HA2	2.07	0.54
2:B:140:GLU:OE1	2:B:162:ARG:NH1	2.38	0.54
2:B:90:ILE:HD13	2:B:296:ILE:HG13	1.88	0.54
1:D:967:GLY:HA3	1:D:975:PHE:CE2	2.43	0.54
1:A:874:VAL:HG11	1:A:916:THR:HG22	1.90	0.54
2:B:257:ILE:HG23	2:B:315:MET:HE1	1.90	0.54
1:D:127:GLU:HB3	1:D:129:ARG:HG3	1.89	0.53
1:D:14:ALA:HB1	1:D:327:ARG:HD2	1.91	0.53
1:A:196:SER:HB2	1:A:199:GLU:HB2	1.91	0.53
1:A:385:GLY:HA3	1:A:719:GLU:O	2.08	0.53
3:C:46:LYS:HE2	3:C:57:LEU:HD11	1.90	0.53
1:D:952:ASN:ND2	1:D:970:ASN:HB3	2.23	0.53
3:F:97:LEU:HD11	3:F:153:LEU:HD21	1.91	0.53
1:A:201:GLU:HG3	1:D:200:LYS:HE2	1.89	0.53
2:B:383:GLY:O	2:B:405:THR:HG23	2.09	0.53
1:D:963:ASP:OD1	1:D:979:LYS:HE3	2.09	0.53
1:A:265:ASP:OD2	1:A:269:SER:HB2	2.09	0.53
1:A:912:LEU:HD11	2:B:244:LEU:HD21	1.91	0.53
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.91	0.53
1:A:725:CYS:SG	1:A:816:LEU:HG	2.49	0.53
1:A:374:GLN:HG2	1:A:391:ARG:HB3	1.91	0.52
2:B:67:PHE:CZ	2:B:114:ILE:HG23	2.44	0.52
2:B:258:LYS:HG2	2:B:273:LEU:HD13	1.89	0.52
1:A:1055:GLN:HG2	1:A:1093:LEU:HD23	1.91	0.52
3:F:238:GLU:O	3:F:242:SER:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:HIS:HD1	2:B:59:TYR:HE1	1.58	0.52
1:D:118:THR:HG22	1:D:118:THR:O	2.10	0.52
1:D:271:TYR:HB2	1:D:283:LEU:HB3	1.91	0.52
2:E:324:LYS:N	2:E:421:ALA:O	2.33	0.52
2:B:107:VAL:HG22	2:B:155:VAL:HG12	1.91	0.52
1:D:366:ASP:HB3	1:D:370:GLN:HA	1.91	0.52
3:F:43:VAL:HG12	3:F:77:ARG:NH1	2.23	0.52
3:C:106:ARG:O	3:C:217:THR:HG22	2.10	0.52
1:D:207:TRP:HB3	1:D:242:GLY:HA2	1.92	0.52
1:D:334:VAL:HA	1:D:349:ALA:HA	1.92	0.52
1:A:84:TYR:CD1	1:A:135:LEU:HD13	2.45	0.51
1:A:108:VAL:O	1:A:141:LYS:HE2	2.10	0.51
1:A:367:LEU:HD12	1:A:374:GLN:NE2	2.26	0.51
2:B:319:THR:HG22	2:B:334:LYS:HE2	1.92	0.51
2:B:326:CYS:C	2:B:328:GLU:H	2.18	0.51
2:B:400:TRP:HZ2	3:C:39:ASN:HA	1.75	0.51
3:F:77:ARG:NH2	3:F:91:ASP:OD1	2.42	0.51
1:D:879:LYS:HB3	1:D:891:TYR:O	2.10	0.51
2:E:353:HIS:CG	3:F:37:ILE:HB	2.45	0.51
1:A:118:THR:OG1	1:A:134:ARG:NH2	2.37	0.51
1:A:765:VAL:HG12	1:A:806:GLN:HB3	1.92	0.51
1:D:324:VAL:HB	1:D:332:GLN:HB2	1.92	0.51
2:B:64:MET:HB3	2:B:144:TYR:O	2.10	0.51
3:F:219:LEU:HD13	3:F:221:TRP:NE1	2.25	0.51
2:B:352:PRO:HG3	2:B:378:HIS:CD2	2.45	0.51
1:D:270:ARG:HG2	1:D:284:LEU:HD23	1.91	0.51
1:D:275:ASP:OD1	1:D:279:ARG:N	2.44	0.51
1:D:364:VAL:HG23	1:D:1008:CYS:SG	2.51	0.51
1:A:335:LYS:HB2	1:A:350:MET:SD	2.50	0.51
1:D:31:LEU:HB3	1:D:42:TYR:HB2	1.93	0.51
1:D:841:ALA:O	2:E:247:LEU:HD21	2.11	0.51
1:D:108:VAL:HB	1:D:141:LYS:HE2	1.93	0.51
2:B:95:GLN:O	2:B:160:ILE:HA	2.11	0.51
1:D:315:THR:HG22	1:D:323:PHE:HB3	1.92	0.51
1:D:952:ASN:CG	1:D:970:ASN:HB3	2.36	0.51
1:D:963:ASP:O	1:D:978:GLN:HA	2.10	0.51
2:E:80:VAL:HA	2:E:180:ALA:O	2.10	0.51
3:F:64:TYR:CE1	3:F:74:PRO:HD2	2.45	0.51
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.46	0.50
2:B:51:THR:O	2:B:54:PRO:HD2	2.11	0.50
3:C:162:LYS:HG2	3:C:163:LYS:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:SER:HB3	1:D:275:ASP:OD2	2.10	0.50
2:B:296:ILE:O	2:B:300:LYS:HG3	2.11	0.50
3:F:144:MET:SD	3:F:153:LEU:HD12	2.52	0.50
1:A:736:LEU:HG	1:A:816:LEU:HD22	1.94	0.50
1:A:922:LEU:HD22	1:A:965:PHE:HD2	1.75	0.50
1:A:812:TYR:CE1	2:B:241:PRO:HG3	2.47	0.50
1:A:935:TYR:O	1:A:937:PRO:HD3	2.10	0.50
1:A:975:PHE:HA	1:A:996:GLY:O	2.12	0.50
1:D:725:CYS:SG	1:D:816:LEU:HG	2.52	0.50
3:F:226:ALA:CB	3:F:231:GLN:HB3	2.41	0.50
1:A:367:LEU:HB2	1:A:374:GLN:HE21	1.76	0.50
1:D:126:PRO:HD3	1:D:169:PHE:HB3	1.93	0.49
2:B:296:ILE:HG22	2:B:300:LYS:HE3	1.94	0.49
3:C:181:LEU:HD23	3:C:233:TYR:CE2	2.47	0.49
1:D:937:PRO:HB2	1:D:938:MET:HE2	1.94	0.49
3:F:197:GLU:HG3	3:F:198:GLN:N	2.27	0.49
3:C:77:ARG:HH11	3:C:77:ARG:HG2	1.77	0.49
1:D:762:SER:O	1:D:803:HIS:HA	2.12	0.49
1:A:198:ARG:NH1	1:D:156:ASN:O	2.46	0.49
1:A:386:SER:HA	1:A:717:LEU:HG	1.95	0.49
1:D:68:ARG:HB2	1:D:75:ASP:OD1	2.13	0.49
2:E:274:PRO:HB2	2:E:279:ASP:HB2	1.94	0.49
3:C:103:PHE:HE2	3:C:301:LEU:HB2	1.77	0.49
3:F:172:HIS:CG	3:F:269:GLU:HG2	2.48	0.49
1:A:245:TYR:CZ	1:A:247:ALA:HB2	2.48	0.49
3:C:185:ALA:HB2	3:C:233:TYR:CE1	2.48	0.49
1:D:258:ILE:HD13	1:D:273:LEU:HD13	1.93	0.49
2:E:352:PRO:HG3	2:E:378:HIS:NE2	2.27	0.49
1:A:753:ARG:HG3	1:A:754:PRO:O	2.12	0.48
3:C:284:LEU:O	3:C:288:LEU:HG	2.13	0.48
1:D:1003:PHE:CE2	2:E:197:VAL:HG22	2.47	0.48
2:B:92:ILE:HG22	2:B:93:PRO:O	2.13	0.48
3:C:25:SER:HA	3:C:30:ASP:HA	1.95	0.48
1:D:49:LEU:HG	1:D:333:LEU:HD11	1.94	0.48
2:E:384:TYR:CD1	2:E:404:ALA:HA	2.49	0.48
3:F:232:LYS:O	3:F:236:ILE:HG13	2.14	0.48
2:B:357:HIS:CD2	2:B:400:TRP:HH2	2.31	0.48
1:D:83:LYS:HE2	1:D:1077:HIS:HB2	1.96	0.48
1:D:828:TYR:HE1	1:D:861:VAL:HG21	1.76	0.48
2:B:165:PHE:HB2	2:B:182:VAL:HG13	1.94	0.48
1:D:282:MET:HB2	1:D:305:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:250:ALA:O	2:E:254:MET:HG3	2.14	0.48
2:E:337:ILE:HG23	2:E:360:LEU:HD11	1.96	0.48
1:A:913:TYR:O	1:A:914:LEU:HD23	2.13	0.48
2:E:384:TYR:HD1	2:E:404:ALA:HA	1.78	0.48
1:D:935:TYR:O	1:D:937:PRO:HD3	2.14	0.47
2:B:48:ASN:OD1	2:B:410:SER:HB3	2.14	0.47
1:A:212:VAL:HG12	1:A:240:HIS:HE1	1.79	0.47
1:A:881:LEU:HD12	1:A:889:ARG:O	2.14	0.47
2:B:408:ASP:OD1	2:B:408:ASP:N	2.45	0.47
1:D:207:TRP:CH2	1:D:228:GLY:HA2	2.49	0.47
1:D:966:LEU:HD12	1:D:975:PHE:O	2.15	0.47
3:F:121:ILE:HD12	3:F:278:ARG:HA	1.97	0.47
1:A:315:THR:CG2	1:A:323:PHE:HB3	2.44	0.47
2:B:109:MET:HE3	2:B:113:LEU:HD11	1.96	0.47
1:A:741:GLU:HG2	1:A:751:ALA:HA	1.97	0.47
1:A:1093:LEU:O	1:A:1096:SER:OG	2.29	0.47
1:D:1098:LEU:HG	1:D:1133:VAL:HG11	1.96	0.47
1:A:312:GLU:OE2	2:B:201:SER:HB3	2.13	0.47
1:A:315:THR:HG23	1:A:323:PHE:HB3	1.97	0.47
2:B:367:ASN:HA	2:B:392:LYS:HD2	1.95	0.47
1:D:143:ILE:HG12	1:D:154:ALA:HB2	1.95	0.47
2:E:119:THR:HA	2:E:139:ALA:O	2.14	0.47
3:F:241:MET:HE2	3:F:241:MET:HB3	1.63	0.47
2:B:102:PHE:CD2	2:B:154:ILE:HD12	2.50	0.47
2:B:197:VAL:HG22	2:B:237:LEU:HD12	1.95	0.47
3:C:125:GLU:O	3:C:129:THR:HG23	2.15	0.47
1:D:1128:ASP:OD1	1:D:1128:ASP:N	2.48	0.47
1:D:58:TYR:HB3	1:D:1073:TRP:CB	2.43	0.47
3:C:194:LEU:HD21	3:C:241:MET:SD	2.55	0.47
2:E:94:GLY:HA2	2:E:160:ILE:HD11	1.97	0.47
1:D:246:LEU:HD11	1:D:299:ASP:HA	1.97	0.46
3:F:102:ASN:OD1	3:F:106:ARG:HD3	2.14	0.46
2:B:165:PHE:CD1	2:B:182:VAL:HG22	2.50	0.46
1:D:313:CYS:SG	1:D:325:GLY:HA3	2.54	0.46
1:A:84:TYR:CE1	1:A:135:LEU:HD13	2.50	0.46
3:C:74:PRO:HG3	3:C:156:ILE:HG22	1.96	0.46
3:F:255:GLU:OE2	3:F:284:LEU:HB2	2.16	0.46
1:A:952:ASN:OD1	1:A:970:ASN:HB3	2.15	0.46
2:E:253:LEU:HD13	2:E:309:ARG:HG3	1.98	0.46
3:F:124:ILE:HD12	3:F:207:LEU:HD22	1.98	0.46
3:C:16:LYS:HE2	3:C:36:ASN:HD21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ILE:HG12	1:A:799:PHE:CZ	2.50	0.46
1:A:310:ILE:HG21	1:A:328:LEU:HD12	1.98	0.46
3:C:237:SER:O	3:C:241:MET:HG3	2.16	0.46
1:D:743:GLN:HB3	1:D:783:GLY:N	2.25	0.46
1:D:889:ARG:HD2	1:D:891:TYR:CZ	2.51	0.46
2:E:81:ILE:O	2:E:180:ALA:N	2.48	0.46
1:A:171:TYR:CG	1:A:223:PRO:HA	2.51	0.46
2:B:315:MET:O	2:B:334:LYS:NZ	2.40	0.46
1:D:1136:LEU:HA	1:D:1139:ILE:HD13	1.96	0.46
2:E:265:ASP:HB2	2:E:339:SER:HB2	1.98	0.46
1:A:166:ASP:HB3	1:A:219:VAL:HG23	1.98	0.46
1:A:793:ILE:HG21	1:A:853:TYR:CD1	2.51	0.46
2:B:149:ASP:O	2:B:152:ILE:HG12	2.15	0.46
1:D:887:THR:HG23	1:D:906:TYR:CD1	2.50	0.46
3:F:199:SER:OG	3:F:201:ARG:HG2	2.16	0.46
1:A:843:PRO:HG2	1:A:869:ALA:HB2	1.96	0.45
1:A:927:MET:HE2	1:A:927:MET:HB3	1.84	0.45
2:B:339:SER:HA	2:B:345:PRO:HA	1.97	0.45
1:D:1076:PHE:O	1:D:1082:THR:HA	2.16	0.45
1:D:387:LEU:HB2	1:D:715:VAL:HB	1.98	0.45
1:D:1080:ARG:H	1:D:1080:ARG:HG2	1.59	0.45
1:A:55:VAL:HG11	1:A:100:ILE:HG13	1.97	0.45
1:A:90:GLU:HB3	1:A:101:ILE:HD11	1.98	0.45
2:E:401:LYS:HB2	2:E:415:TRP:CZ3	2.52	0.45
1:A:815:SER:OG	1:A:873:MET:HE2	2.17	0.45
1:A:912:LEU:CD2	2:B:244:LEU:HD11	2.45	0.45
2:B:412:GLN:HE21	2:B:412:GLN:HB2	1.56	0.45
1:D:315:THR:CG2	1:D:323:PHE:HB3	2.47	0.45
2:E:288:LEU:C	2:E:346:MET:HE1	2.42	0.45
1:D:1057:ARG:O	1:D:1061:VAL:HG13	2.17	0.45
3:F:263:CYS:HA	3:F:266:LEU:HD12	1.99	0.45
3:F:275:MET:CE	3:F:278:ARG:HH21	2.29	0.45
1:A:1027:SER:OG	1:A:1039:LEU:HD11	2.17	0.45
1:A:271:TYR:HB2	1:A:283:LEU:HB3	1.99	0.45
1:D:207:TRP:HB2	1:D:242:GLY:HA2	1.98	0.45
1:D:267:ASN:ND2	1:D:269:SER:OG	2.49	0.45
1:D:1109:VAL:O	1:D:1110:ALA:C	2.59	0.45
3:F:160:LEU:HD13	3:F:182:THR:HG22	1.99	0.45
1:A:218:MET:HE3	1:A:218:MET:HB2	1.83	0.44
3:C:212:MET:HE1	3:C:252:PHE:CD2	2.53	0.44
2:E:388:VAL:HG21	3:F:41:GLU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:25:SER:HA	3:F:30:ASP:HA	1.98	0.44
2:B:303:SER:HB3	2:B:306:GLN:HG3	1.99	0.44
3:C:39:ASN:OD1	3:C:41:GLU:HB3	2.17	0.44
2:E:135:PHE:N	2:E:135:PHE:CD1	2.85	0.44
1:D:952:ASN:OD1	1:D:970:ASN:HB3	2.17	0.44
2:E:250:ALA:HB2	2:E:305:ILE:HD11	1.99	0.44
3:F:21:ARG:HG3	3:F:23:ILE:HG23	2.00	0.44
3:F:117:ALA:O	3:F:121:ILE:HG13	2.17	0.44
1:A:367:LEU:HB2	1:A:374:GLN:NE2	2.33	0.44
2:B:294:LEU:HD23	2:B:294:LEU:HA	1.86	0.44
1:D:40:GLU:HB3	1:D:42:TYR:HE1	1.81	0.44
2:E:89:MET:SD	2:E:97:LEU:HD13	2.57	0.44
3:F:50:GLN:HG3	3:F:84:ASP:O	2.17	0.44
3:F:137:ILE:HG22	3:F:210:VAL:HG21	1.99	0.44
3:F:191:ASN:HB3	3:F:196:ILE:HD12	1.99	0.44
1:D:180:PHE:CE1	1:D:191:LYS:HB3	2.52	0.44
1:A:388:ARG:NE	1:A:714:THR:HG23	2.33	0.44
3:C:46:LYS:HE3	3:C:46:LYS:HB3	1.82	0.44
3:C:122:SER:OG	3:C:278:ARG:NH1	2.51	0.44
1:D:190:VAL:HG12	1:D:210:GLU:H	1.83	0.44
1:A:80:LEU:HD12	1:A:85:ASN:O	2.17	0.44
1:A:869:ALA:O	1:A:884:ILE:HA	2.18	0.44
2:B:84:LEU:HD12	2:B:120:PHE:CE2	2.52	0.44
1:D:321:VAL:HG22	1:D:350:MET:SD	2.58	0.44
1:D:916:THR:CG2	1:D:921:ILE:HG13	2.44	0.44
2:E:339:SER:HA	2:E:345:PRO:HA	1.99	0.44
1:A:333:LEU:HB2	1:A:351:GLU:HB2	2.00	0.44
3:C:15:GLY:O	3:C:37:ILE:HD11	2.18	0.44
1:D:1014:MET:HE3	1:D:1014:MET:HB2	1.68	0.44
2:E:74:ASP:O	2:E:77:SER:HB3	2.18	0.44
2:E:77:SER:OG	2:E:79:GLN:OE1	2.35	0.44
1:D:1030:PHE:CZ	1:D:1038:GLY:HA3	2.53	0.43
1:A:270:ARG:HE	1:A:270:ARG:HB2	1.73	0.43
3:F:239:LYS:O	3:F:243:THR:OG1	2.25	0.43
1:A:18:CYS:HA	1:A:32:LEU:O	2.18	0.43
1:D:166:ASP:HB3	1:D:219:VAL:HG23	1.99	0.43
1:D:741:GLU:HG2	1:D:751:ALA:HA	2.00	0.43
1:A:213:GLU:HG2	1:A:215:GLU:H	1.84	0.43
1:A:866:VAL:HG21	1:A:884:ILE:HG12	2.00	0.43
2:B:71:THR:HG21	2:B:117:ASP:HB2	2.00	0.43
1:D:1058:LEU:HD21	1:D:1097:PHE:CD1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:353:HIS:CD2	3:F:37:ILE:HB	2.53	0.43
1:D:250:PRO:HB2	1:D:252:ILE:HG22	2.01	0.43
1:D:928:ARG:HB2	1:D:952:ASN:O	2.18	0.43
2:E:371:ILE:HG21	3:F:41:GLU:HG3	1.99	0.43
2:B:247:LEU:O	2:B:309:ARG:HD2	2.19	0.43
3:C:16:LYS:HA	3:C:37:ILE:HG12	1.99	0.43
3:F:279:GLN:O	3:F:283:ILE:HG13	2.19	0.43
1:D:893:TRP:HA	1:D:893:TRP:CE3	2.52	0.43
2:B:378:HIS:O	5:B:502:YOT:N26	2.52	0.43
1:D:84:TYR:CE1	1:D:135:LEU:HD13	2.53	0.43
1:D:812:TYR:CZ	2:E:241:PRO:HB3	2.54	0.43
1:D:927:MET:HE3	2:E:190:LEU:HD12	2.00	0.43
2:E:373:ARG:NE	3:F:146:ILE:HG23	2.34	0.43
2:B:349:TYR:O	2:B:356:VAL:HA	2.19	0.43
3:F:181:LEU:HB3	3:F:233:TYR:HE2	1.83	0.43
1:A:16:ASN:HA	1:A:312:GLU:HG2	2.00	0.43
2:B:75:ASP:O	2:B:76:ASP:HB2	2.19	0.43
3:C:259:TYR:CE1	3:C:277:LEU:HD13	2.53	0.43
1:D:218:MET:HB2	1:D:218:MET:HE3	1.78	0.43
1:D:1139:ILE:HG12	1:D:1140:HIS:N	2.34	0.43
1:A:793:ILE:HG21	1:A:853:TYR:CE1	2.54	0.42
2:B:92:ILE:O	2:B:95:GLN:HB2	2.19	0.42
2:B:169:GLU:O	2:B:181:LYS:N	2.50	0.42
3:C:126:TYR:OH	3:C:130:LYS:HE3	2.18	0.42
1:D:308:THR:HB	1:D:332:GLN:OE1	2.18	0.42
1:D:805:HIS:CD2	1:D:806:GLN:O	2.72	0.42
1:D:835:MET:HB3	1:D:837:TYR:CE1	2.54	0.42
2:E:397:HIS:HE1	2:E:400:TRP:CZ2	2.37	0.42
1:A:952:ASN:CG	1:A:970:ASN:HB3	2.44	0.42
3:C:16:LYS:HE2	3:C:36:ASN:ND2	2.34	0.42
1:D:1105:MET:O	1:D:1109:VAL:HG13	2.19	0.42
2:E:368:LEU:O	2:E:392:LYS:NZ	2.51	0.42
1:A:388:ARG:CZ	1:A:714:THR:HG23	2.49	0.42
1:A:1058:LEU:HD22	1:A:1062:ILE:HD11	2.01	0.42
1:D:876:PHE:CE2	1:D:921:ILE:HD11	2.55	0.42
1:A:819:CYS:HB2	1:A:875:GLU:HG3	2.00	0.42
1:A:828:TYR:CE1	1:A:861:VAL:HG21	2.53	0.42
1:D:194:GLU:HB2	1:D:203:ASN:HB2	2.01	0.42
1:D:928:ARG:O	1:D:930:VAL:HG23	2.19	0.42
1:A:39:LEU:HB3	1:A:55:VAL:HG23	2.02	0.42
1:D:132:GLY:O	1:D:133:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:999:HIS:HB3	1:D:1074:ARG:HA	2.02	0.42
3:F:57:LEU:HD23	3:F:57:LEU:HA	1.80	0.42
2:B:84:LEU:HG	2:B:109:MET:HE1	2.01	0.42
2:B:123:LEU:HB2	2:B:125:TYR:CZ	2.54	0.42
3:C:114:LEU:HD23	3:C:114:LEU:HA	1.87	0.42
1:D:141:LYS:HB2	1:D:156:ASN:OD1	2.19	0.42
1:A:762:SER:O	1:A:803:HIS:HA	2.20	0.42
1:D:134:ARG:NH1	1:D:164:VAL:O	2.50	0.42
2:E:244:LEU:O	2:E:244:LEU:HG	2.12	0.42
1:A:795:ASP:OD2	1:A:798:THR:HG23	2.20	0.42
2:B:198:GLN:HA	2:B:234:CYS:SG	2.60	0.42
2:B:290:ILE:HD12	2:B:294:LEU:HB3	2.01	0.42
3:C:201:ARG:CZ	3:C:268:PHE:HA	2.49	0.42
1:D:1054:MET:O	1:D:1058:LEU:HD12	2.20	0.42
3:F:123:ARG:O	3:F:127:VAL:HG23	2.19	0.42
1:A:812:TYR:CZ	2:B:241:PRO:HB3	2.55	0.42
1:A:978:GLN:O	1:A:992:LEU:HA	2.20	0.42
3:C:57:LEU:HD12	3:C:57:LEU:HA	1.78	0.42
2:E:135:PHE:HD1	2:E:135:PHE:H	1.66	0.42
2:B:209:PRO:C	2:B:223:TRP:HE1	2.27	0.42
3:C:193:HIS:C	3:C:195:GLY:H	2.28	0.42
3:C:246:GLU:OE1	3:C:246:GLU:N	2.50	0.42
1:D:126:PRO:HB3	1:D:171:TYR:CE1	2.54	0.42
1:D:931:LEU:HD12	1:D:947:ARG:HB3	2.02	0.41
2:E:373:ARG:NH2	3:F:147:GLY:H	2.18	0.41
3:F:212:MET:HE1	3:F:252:PHE:CD2	2.55	0.41
1:A:375:LEU:HD23	1:A:1037:ILE:HD13	2.02	0.41
1:A:963:ASP:O	1:A:978:GLN:HA	2.19	0.41
1:D:182:TYR:O	1:D:188:ARG:HA	2.20	0.41
1:D:843:PRO:CG	1:D:869:ALA:HB2	2.50	0.41
2:E:118:ARG:O	2:E:140:GLU:HA	2.20	0.41
1:A:951:PRO:O	2:B:190:LEU:HD21	2.19	0.41
1:D:926:LEU:HD21	2:E:245:TYR:CD1	2.56	0.41
1:A:30:ASN:HA	1:A:42:TYR:O	2.20	0.41
1:A:105:HIS:CD2	1:A:1067:LYS:HD2	2.55	0.41
1:A:998:PHE:HB2	1:A:1088:PHE:CD2	2.54	0.41
3:C:76:ILE:HD13	3:C:76:ILE:HA	1.88	0.41
1:D:166:ASP:OD2	1:D:219:VAL:N	2.47	0.41
1:A:1054:MET:SD	1:A:1129:LEU:HD21	2.60	0.41
1:D:143:ILE:CG1	1:D:154:ALA:HB2	2.50	0.41
1:D:376:VAL:HA	1:D:388:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:HD3	1:A:38:ARG:HD2	2.03	0.41
2:B:89:MET:HE1	2:B:91:LEU:HD13	2.03	0.41
2:B:165:PHE:HA	2:B:185:LEU:HG	2.01	0.41
2:B:347:ALA:HB3	2:B:349:TYR:CZ	2.56	0.41
1:D:42:TYR:CD2	1:D:49:LEU:HB3	2.55	0.41
1:D:317:LEU:HD12	1:D:321:VAL:HG12	2.03	0.41
1:A:226:PHE:O	1:A:241:ASN:ND2	2.54	0.41
1:A:853:TYR:CZ	1:A:856:GLY:HA2	2.56	0.41
1:D:736:LEU:HG	1:D:816:LEU:HD22	2.03	0.41
2:E:277:PRO:O	2:E:304:ALA:HB1	2.21	0.41
2:E:281:SER:OG	2:E:307:ARG:HD2	2.21	0.41
1:A:923:VAL:HB	1:A:931:LEU:HB3	2.02	0.41
2:B:306:GLN:HG3	2:B:306:GLN:H	1.70	0.41
1:D:798:THR:OG1	1:D:800:GLU:HG2	2.21	0.41
2:E:291:ASP:OD1	2:E:291:ASP:N	2.54	0.41
3:F:116:LEU:HD23	3:F:116:LEU:HA	1.86	0.41
1:A:102:THR:HB	1:A:1067:LYS:HE3	2.03	0.41
1:A:132:GLY:O	1:A:133:LEU:HD23	2.21	0.41
1:A:912:LEU:HA	1:A:912:LEU:HD23	1.69	0.41
2:B:99:LEU:HA	2:B:99:LEU:HD23	1.62	0.41
1:D:916:THR:HG22	1:D:921:ILE:HA	2.02	0.41
2:E:401:LYS:HB2	2:E:415:TRP:CE3	2.55	0.41
3:F:50:GLN:HG3	3:F:84:ASP:C	2.46	0.41
1:A:1129:LEU:O	1:A:1133:VAL:HG23	2.21	0.41
2:B:127:ASN:HB3	2:B:130:GLU:CB	2.51	0.41
1:D:64:MET:HG2	1:D:77:LEU:HD11	2.03	0.41
1:D:130:MET:HE3	1:D:176:PRO:HG2	2.03	0.41
1:D:333:LEU:O	1:D:350:MET:N	2.54	0.41
3:F:95:PRO:HG2	3:F:100:LEU:HD21	2.03	0.41
3:F:142:PHE:HB3	3:F:153:LEU:HD21	2.03	0.40
1:A:928:ARG:NH2	1:A:948:ASP:OD2	2.55	0.40
3:C:115:MET:HE3	3:C:296:PHE:CD1	2.57	0.40
1:D:24:THR:HA	1:D:91:TYR:CD2	2.57	0.40
1:D:142:VAL:HB	1:D:155:PHE:CZ	2.57	0.40
1:D:756:ALA:HB1	1:D:801:VAL:HG21	2.03	0.40
1:D:1000:LEU:HD21	1:D:1030:PHE:CE1	2.56	0.40
3:F:271:ALA:HA	3:F:272:PRO:HD3	1.97	0.40
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	2.04	0.40
2:E:91:LEU:HB3	2:E:137:THR:HG21	2.03	0.40
3:F:185:ALA:O	3:F:186:ARG:C	2.65	0.40
1:A:971:ALA:HB3	1:A:1077:HIS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLU:O	2:B:143:ALA:HA	2.21	0.40
1:D:359:ILE:HG21	1:D:1031:GLY:HA3	2.04	0.40
3:F:244:PRO:HD2	3:F:247:VAL:CG2	2.52	0.40
2:B:322:CYS:HB3	2:B:329:THR:O	2.22	0.40
1:D:291:MET:HB3	1:D:291:MET:HE3	1.62	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	764/860 (89%)	730 (96%)	34 (4%)	0	100	100
1	D	765/860 (89%)	732 (96%)	33 (4%)	0	100	100
2	B	368/426 (86%)	362 (98%)	6 (2%)	0	100	100
2	E	289/426 (68%)	281 (97%)	8 (3%)	0	100	100
3	C	283/341 (83%)	264 (93%)	19 (7%)	0	100	100
3	F	292/341 (86%)	276 (94%)	16 (6%)	0	100	100
All	All	2761/3254 (85%)	2645 (96%)	116 (4%)	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	575/746 (77%)	555 (96%)	20 (4%)	32	58
1	D	604/746 (81%)	563 (93%)	41 (7%)	14	41
2	B	293/385 (76%)	274 (94%)	19 (6%)	15	43
2	E	203/385 (53%)	189 (93%)	14 (7%)	14	41
3	C	233/293 (80%)	219 (94%)	14 (6%)	17	45
3	F	246/293 (84%)	233 (95%)	13 (5%)	20	48
All	All	2154/2848 (76%)	2033 (94%)	121 (6%)	19	47

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ILE
1	A	117	GLU
1	A	127	GLU
1	A	141	LYS
1	A	215	GLU
1	A	259	VAL
1	A	270	ARG
1	A	360	VAL
1	A	376	VAL
1	A	720	SER
1	A	730	SER
1	A	752	LEU
1	A	768	SER
1	A	790	ASN
1	A	928	ARG
1	A	962	ASP
1	A	979	LYS
1	A	1006	VAL
1	A	1032	THR
1	A	1033	VAL
2	B	52	SER
2	B	53	LEU
2	B	56	SER
2	B	75	ASP
2	B	92	ILE
2	B	95	GLN
2	B	149	ASP
2	B	157	VAL
2	B	162	ARG
2	B	177	ILE

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Mol	Chain	Res	Type
2	B	182	VAL
2	B	193	THR
2	B	194	MET
2	B	238	THR
2	B	242	ARG
2	B	351	ASN
2	B	377	GLU
2	B	378	HIS
2	B	405	THR
3	C	16	LYS
3	C	18	LYS
3	C	23	ILE
3	C	31	ILE
3	C	35	ILE
3	C	41	GLU
3	C	47	LEU
3	C	63	LEU
3	C	68	GLN
3	C	71	VAL
3	C	96	SER
3	C	184	THR
3	C	216	ARG
3	C	245	VAL
1	D	89	LEU
1	D	127	GLU
1	D	139	LEU
1	D	141	LYS
1	D	148	ASP
1	D	153	LYS
1	D	184	ASP
1	D	190	VAL
1	D	192	THR
1	D	222	VAL
1	D	231	ILE
1	D	232	ILE
1	D	275	ASP
1	D	352	THR
1	D	354	THR
1	D	720	SER
1	D	752	LEU
1	D	762	SER
1	D	792	LEU

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Mol	Chain	Res	Type
1	D	815	SER
1	D	873	MET
1	D	874	VAL
1	D	875	GLU
1	D	887	THR
1	D	892	GLU
1	D	894	THR
1	D	895	THR
1	D	897	LYS
1	D	900	ARG
1	D	928	ARG
1	D	962	ASP
1	D	1006	VAL
1	D	1014	MET
1	D	1032	THR
1	D	1061	VAL
1	D	1080	ARG
1	D	1125	THR
1	D	1128	ASP
1	D	1133	VAL
1	D	1134	GLU
1	D	1139	ILE
2	E	79	GLN
2	E	81	ILE
2	E	87	VAL
2	E	96	THR
2	E	135	PHE
2	E	137	THR
2	E	160	ILE
2	E	182	VAL
2	E	184	ILE
2	E	197	VAL
2	E	266	GLU
2	E	298	LEU
2	E	300	LYS
2	E	379	SER
3	F	13	VAL
3	F	30	ASP
3	F	31	ILE
3	F	71	VAL
3	F	73	ILE
3	F	153	LEU

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Mol	Chain	Res	Type
3	F	156	ILE
3	F	197	GLU
3	F	216	ARG
3	F	222	GLN
3	F	231	GLN
3	F	235	LYS
3	F	242	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	189	HIS
1	A	261	HIS
1	A	859	GLN
1	A	885	ASN
1	A	964	ASN
2	B	79	GLN
2	B	100	GLN
3	C	50	GLN
3	C	151	ASN
3	C	198	GLN
3	C	289	ASN
3	C	290	HIS
1	D	203	ASN
1	D	727	GLN
1	D	759	GLN
1	D	790	ASN
1	D	970	ASN
2	E	306	GLN
2	E	316	ASN
2	E	335	ASN
2	E	369	ASN
3	F	50	GLN
3	F	141	ASN
3	F	149	HIS
3	F	290	HIS

5.3.3 RNA ⓘ

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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
5	YOT	B	502	-	32,32,32	0.56	1 (3%)	45,47,47	1.21	3 (6%)

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
5	YOT	B	502	-	-	0/8/33/33	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	YOT	C10-N11	2.11	1.30	1.29

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	YOT	O12-N11-C10	5.06	107.66	104.15
5	B	502	YOT	C15-C14-C10	3.05	136.76	131.38
5	B	502	YOT	C02-C03-N04	-2.17	108.31	110.32

There are no chirality outliers.

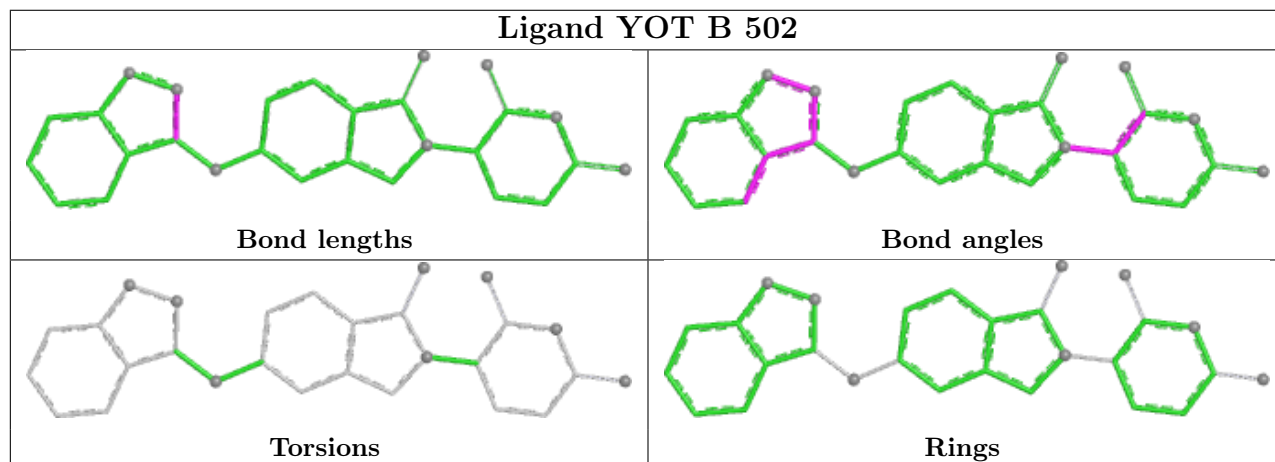
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	YOT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	778/860 (90%)	-0.02	13 (1%)	69 44	74, 129, 191, 243	0
1	D	779/860 (90%)	-0.01	10 (1%)	75 51	62, 117, 181, 256	0
2	B	372/426 (87%)	-0.00	6 (1%)	70 46	82, 114, 199, 304	0
2	E	303/426 (71%)	0.05	5 (1%)	69 44	87, 147, 196, 253	0
3	C	289/341 (84%)	-0.19	3 (1%)	79 56	78, 109, 162, 202	0
3	F	294/341 (86%)	-0.20	3 (1%)	79 56	66, 98, 149, 195	0
All	All	2815/3254 (86%)	-0.05	40 (1%)	73 49	62, 119, 188, 304	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	197	VAL	4.1
1	A	122	GLY	3.1
1	D	122	GLY	3.0
2	B	193	THR	2.9
3	C	14	GLY	2.9
3	F	184	THR	2.8
2	E	167	VAL	2.6
1	D	955	SER	2.5
2	E	381	PHE	2.5
1	D	132	GLY	2.4
2	E	74	ASP	2.4
1	D	135	LEU	2.4
2	E	189	VAL	2.4
1	A	132	GLY	2.4
1	D	62	ALA	2.4
1	A	945	ILE	2.3
1	A	142	VAL	2.3
1	A	123	ILE	2.3
1	A	949	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	338	VAL	2.3
2	E	134	GLN	2.3
1	A	763	SER	2.2
1	A	855	ASP	2.2
3	F	303	GLN	2.2
1	D	368	GLU	2.2
1	D	1023	PRO	2.2
2	B	205	CYS	2.2
3	C	185	ALA	2.2
1	A	961	ASP	2.2
3	C	291	GLN	2.2
1	A	339	ASP	2.1
2	B	318	CYS	2.1
2	B	294	LEU	2.1
1	D	978	GLN	2.1
1	A	179	CYS	2.1
1	A	1079	GLU	2.1
3	F	63	LEU	2.0
1	D	367	LEU	2.0
2	B	415	TRP	2.0
1	D	121	ILE	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.

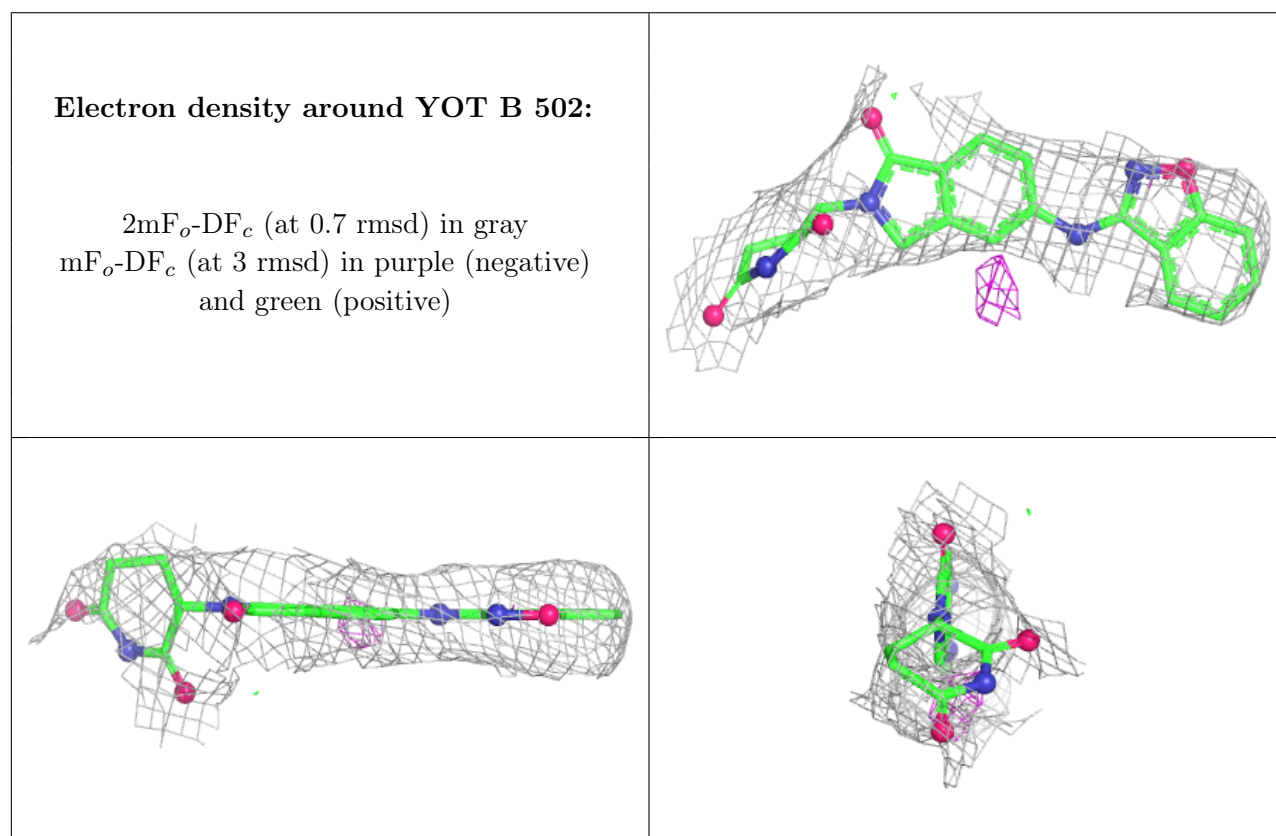
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	YOT	B	502	28/28	0.93	0.09	80,94,117,118	0
4	ZN	E	501	1/1	1.00	0.02	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	B	501	1/1	1.00	0.01	110,110,110,110	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.