



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:01 PM UTC

PDB ID : 8BU5 / pdb_00008bu5
Title : Structure of DDB1 bound to SR-4835-engaged CDK12-cyclin K
Authors : Kozicka, Z.; Kempf, G.; Petzold, G.; Thoma, N.H.
Deposited on : 2022-11-30
Resolution : 3.13 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:

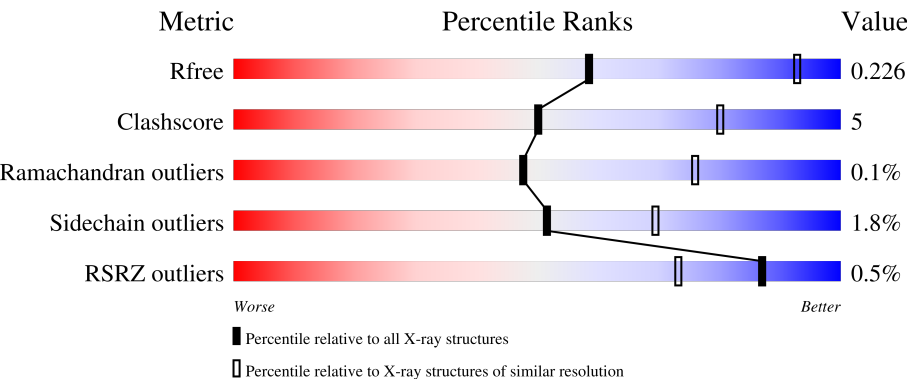
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	840	82%16%.
1	D	840	87%11%.
1	G	840	% 80%18%.
2	B	344	% 78%17%. .
2	E	344	% 77%18%. .

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Mol	Chain	Length	Quality of chain
2	H	344	% 84% 11% . .
3	C	271	85% 7% 8%
3	F	271	83% 8% 8%
3	I	271	86% 6% 8%

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
6	CIT	I	301	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 67681 atoms, of which 33741 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	826	Total	C	H	N	O	S	6485	0	0
			12936	4105	6449	1094	1252	36			
1	D	827	Total	C	H	N	O	S	6462	0	0
			12957	4111	6462	1095	1253	36			
1	G	826	Total	C	H	N	O	S	6452	0	0
			12938	4106	6452	1093	1251	36			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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	-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
G	-3	GLY	-	expression tag	UNP Q16531
G	-2	GLY	-	expression tag	UNP Q16531
G	-1	GLY	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	ARG	-	expression tag	UNP Q16531
G	700	GLY	-	linker	UNP Q16531
G	701	ASN	-	linker	UNP Q16531
G	702	GLY	-	linker	UNP Q16531
G	703	ASN	-	linker	UNP Q16531
G	704	SER	-	linker	UNP Q16531
G	705	GLY	-	linker	UNP Q16531

- Molecule 2 is a protein called Cyclin-dependent kinase 12.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	B	332	Total	C	H	N	O	P	S	2723	0	0
			5436	1737	2723	461	497	1	17			
2	E	331	Total	C	H	N	O	P	S	2718	0	0
			5425	1734	2718	460	495	1	17			
2	H	331	Total	C	H	N	O	P	S	2718	0	0
			5425	1734	2718	460	495	1	17			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	709	GLY	-	expression tag	UNP Q9NYV4
B	710	GLY	-	expression tag	UNP Q9NYV4
B	711	GLY	-	expression tag	UNP Q9NYV4
B	965	ARG	LYS	engineered mutation	UNP Q9NYV4
B	1052	GLN	-	expression tag	UNP Q9NYV4
E	709	GLY	-	expression tag	UNP Q9NYV4
E	710	GLY	-	expression tag	UNP Q9NYV4
E	711	GLY	-	expression tag	UNP Q9NYV4
E	965	ARG	LYS	engineered mutation	UNP Q9NYV4
E	1052	GLN	-	expression tag	UNP Q9NYV4
H	709	GLY	-	expression tag	UNP Q9NYV4
H	710	GLY	-	expression tag	UNP Q9NYV4
H	711	GLY	-	expression tag	UNP Q9NYV4
H	965	ARG	LYS	engineered mutation	UNP Q9NYV4
H	1052	GLN	-	expression tag	UNP Q9NYV4

- Molecule 3 is a protein called Cyclin-K.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
3	C	248	Total	C	H	N	O	S		2048	0	0
			4111	1341	2048	346	363	13				

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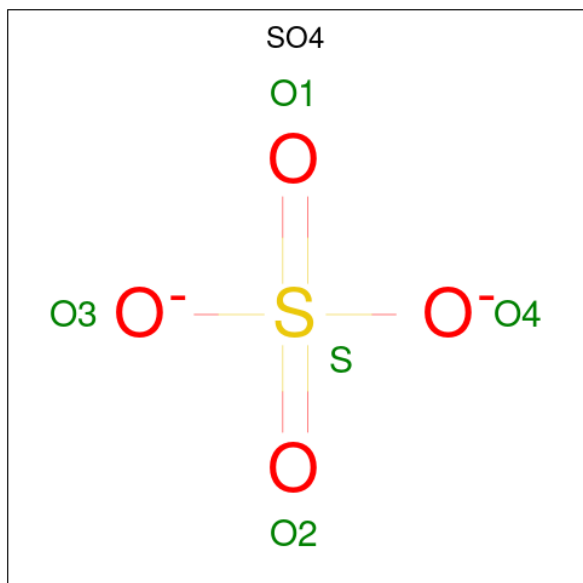
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			
3	I	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP O75909
C	-2	GLY	-	expression tag	UNP O75909
C	-1	GLY	-	expression tag	UNP O75909
C	0	ARG	-	expression tag	UNP O75909
F	-3	GLY	-	expression tag	UNP O75909
F	-2	GLY	-	expression tag	UNP O75909
F	-1	GLY	-	expression tag	UNP O75909
F	0	ARG	-	expression tag	UNP O75909
I	-3	GLY	-	expression tag	UNP O75909
I	-2	GLY	-	expression tag	UNP O75909
I	-1	GLY	-	expression tag	UNP O75909
I	0	ARG	-	expression tag	UNP O75909

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



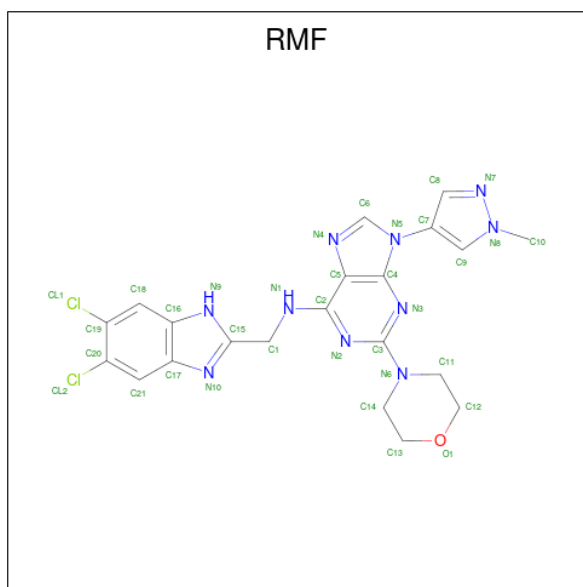
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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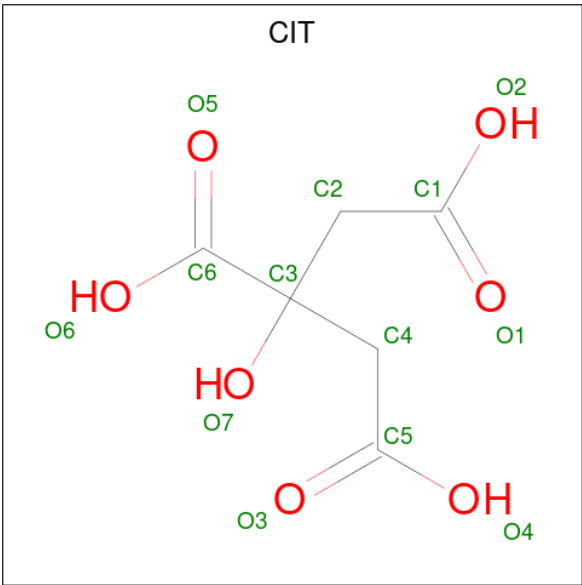
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is {N}-[[5,6-bis(chloranyl)-1 {H}-benzimidazol-2-yl]methyl]-9-(1-methylpyrazol-4-yl)-2-morpholin-4-yl-purin-6-amine (CCD ID: RMF) (formula: C₂₁H₂₀Cl₂N₁₀O) (labeled as "Ligand of Interest" by depositor).

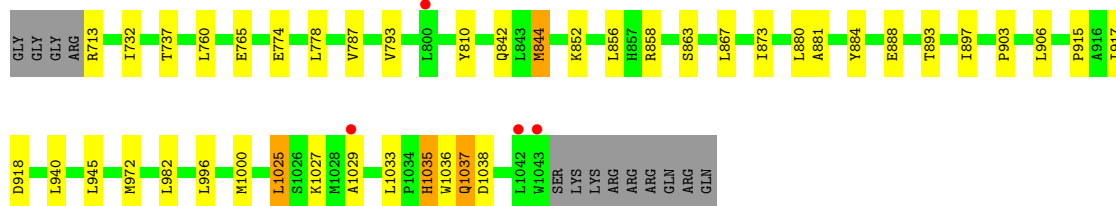
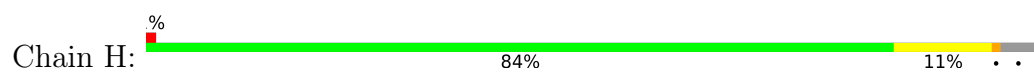


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	Cl	H	N	O	20	0
			54	21	2	20	10	1		
5	E	1	Total	C	Cl	H	N	O	20	0
			54	21	2	20	10	1		
5	H	1	Total	C	Cl	H	N	O	20	0
			54	21	2	20	10	1		

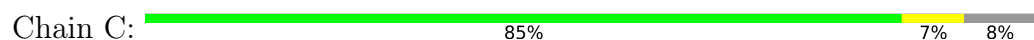
- Molecule 6 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



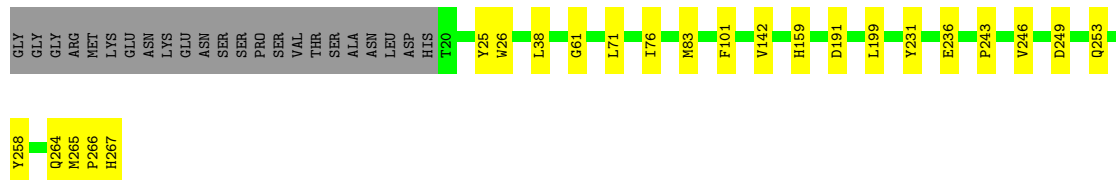
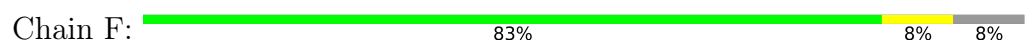
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	H	O	5	0
			18	6	5	7		
6	F	1	Total	C	H	O	5	0
			18	6	5	7		
6	I	1	Total	C	H	O	5	0
			18	6	5	7		



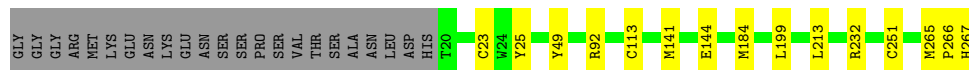
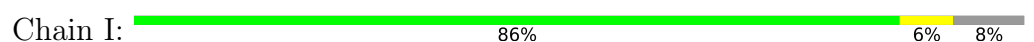
• Molecule 3: Cyclin-K



• Molecule 3: Cyclin-K



• Molecule 3: Cyclin-K



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	249.94Å 249.94Å 219.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.58 – 3.13 60.58 – 3.13	Depositor EDS
% Data completeness (in resolution range)	78.2 (60.58-3.13) 78.2 (60.58-3.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.199 , 0.220 0.206 , 0.226	Depositor DCC
R_{free} test set	5407 reflections (3.91%)	wwPDB-VP
Wilson B-factor (Å ²)	121.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 90.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	67681	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: TPO, RMF, SO4, CIT

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	0.30	0/6604	0.58	0/8931
1	D	0.28	0/6612	0.56	0/8942
1	G	0.32	0/6603	0.60	0/8930
2	B	0.33	0/2763	0.59	0/3725
2	E	0.34	0/2757	0.61	0/3717
2	H	0.36	0/2757	0.64	0/3717
3	C	0.28	0/2120	0.49	0/2868
3	F	0.30	0/2120	0.52	0/2868
3	I	0.29	0/2120	0.50	0/2868
All	All	0.31	0/34456	0.58	0/46566

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6487	6449	6451	79	0
1	D	6495	6462	6464	52	1
1	G	6486	6452	6454	93	0
2	B	2713	2723	2723	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2707	2718	2718	39	1
2	H	2707	2718	2718	30	1
3	C	2063	2048	2048	13	0
3	F	2063	2048	2048	12	0
3	I	2063	2048	2048	8	1
4	A	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
5	B	34	20	0	0	0
5	E	34	20	0	1	0
5	H	34	20	0	0	0
6	C	13	5	5	0	0
6	F	13	5	5	0	0
6	I	13	5	5	0	0
All	All	33940	33741	33687	358	2

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 5.

All (358) 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:C:52:GLU:OE1	3:C:92:ARG:NH1	2.12	0.82
1:A:1109:VAL:HG12	1:A:1129:LEU:HD12	1.67	0.77
1:G:768:SER:HB3	1:G:808:LEU:HD11	1.70	0.74
3:F:231:TYR:OH	3:F:236:GLU:OE1	2.05	0.73
1:G:387:LEU:HG	1:G:717:LEU:HD11	1.71	0.72
1:G:1047:TRP:HZ3	1:G:1132:VAL:HG13	1.57	0.70
3:F:191:ASP:OD2	3:F:258:TYR:OH	2.05	0.69
2:B:835:HIS:HD2	2:B:1029:ALA:HB1	1.57	0.69
2:B:1035:HIS:CG	2:B:1036:TRP:H	2.11	0.69
2:B:1036:TRP:HA	2:B:1036:TRP:CE3	2.27	0.69
1:D:925:ASP:OD1	1:D:926:LEU:N	2.26	0.69
1:A:1098:LEU:HD21	1:A:1133:VAL:HB	1.77	0.67
2:B:856:LEU:HD11	2:B:915:PRO:HG3	1.77	0.67
1:G:270:ARG:HG2	1:G:284:LEU:HD23	1.76	0.67
2:E:839:PHE:HA	2:E:873:ILE:HD13	1.76	0.66
1:D:248:ILE:HD12	1:D:300:LEU:O	1.97	0.65
2:B:1034:PRO:HB2	2:B:1038:ASP:OD1	1.97	0.65
2:H:713:ARG:HG3	3:I:23:CYS:H	1.61	0.63
2:E:871:GLY:C	2:E:1028:MET:HE2	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HB2	1:A:321:VAL:HG23	1.81	0.62
2:B:835:HIS:CD2	2:B:1029:ALA:HB1	2.33	0.62
1:G:311:ALA:HB2	1:G:324:VAL:HG13	1.80	0.62
2:B:856:LEU:HD13	2:B:884:TYR:HB2	1.81	0.61
1:G:127:GLU:HB2	1:G:129:ARG:HG3	1.82	0.61
1:A:246:LEU:HD11	1:A:299:ASP:HA	1.81	0.61
1:A:1109:VAL:HG11	1:A:1126:ALA:HA	1.83	0.61
1:G:230:ILE:HD13	1:G:283:LEU:HD21	1.83	0.60
2:H:842:GLN:HG3	2:H:1025:LEU:HD11	1.83	0.60
1:G:263:ARG:HB3	1:G:271:TYR:CE1	2.36	0.60
1:D:709:LYS:HG2	1:D:710:LEU:H	1.66	0.60
2:B:1036:TRP:HA	2:B:1036:TRP:HE3	1.65	0.60
1:D:770:LEU:HD13	1:D:865:GLU:HB2	1.83	0.60
2:H:888:GLU:HA	2:H:888:GLU:OE1	2.00	0.60
1:A:286:GLU:O	1:A:297:LEU:HD12	2.01	0.60
2:H:856:LEU:HD13	2:H:884:TYR:HB2	1.83	0.59
2:B:844:MET:HE1	2:B:922:CYS:CB	2.32	0.59
1:G:773:SER:C	1:G:775:THR:H	2.10	0.59
2:B:829:VAL:HG12	2:B:1033:LEU:HD23	1.85	0.59
1:D:230:ILE:HD11	1:D:285:LEU:HD21	1.83	0.58
1:A:1106:GLN:HA	1:A:1109:VAL:HG22	1.85	0.58
1:D:228:GLY:HA3	1:D:241:ASN:HB2	1.84	0.58
1:A:226:PHE:CZ	1:A:287:LYS:HG2	2.39	0.58
1:A:949:PHE:HZ	2:B:732:ILE:HG23	1.70	0.57
2:B:889:SER:HB2	2:B:912:ARG:HG2	1.87	0.57
1:G:69:PRO:HD2	1:G:72:GLU:HG3	1.86	0.56
1:A:7:VAL:HG12	1:A:1091:GLY:HA3	1.87	0.56
2:E:856:LEU:HD11	2:E:915:PRO:HG3	1.87	0.56
1:G:715:VAL:HG11	1:G:799:PHE:HB3	1.86	0.56
1:G:830:ILE:HG12	1:G:850:VAL:HG13	1.87	0.56
1:G:223:PRO:HD3	1:G:271:TYR:OH	2.04	0.56
2:E:742:TYR:HB2	2:E:755:LEU:HD12	1.86	0.56
3:I:113:CYS:HB2	3:I:141:MET:HE2	1.87	0.56
1:A:248:ILE:HG21	1:A:300:LEU:O	2.05	0.55
1:G:72:GLU:OE2	1:G:103:ARG:NH2	2.39	0.55
1:G:297:LEU:HD21	1:G:300:LEU:HD21	1.87	0.55
1:D:213:GLU:HG2	1:D:215:GLU:H	1.71	0.55
1:G:19:VAL:HG22	1:G:64:MET:HE3	1.88	0.55
2:B:844:MET:HE1	2:B:922:CYS:HB2	1.87	0.55
1:G:1127:ASP:O	1:G:1131:LYS:HG2	2.07	0.55
1:A:311:ALA:HB2	1:A:324:VAL:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:985:THR:HG22	1:G:987:GLU:H	1.72	0.55
1:A:1133:VAL:O	1:A:1137:THR:HG23	2.07	0.54
1:A:1135:GLU:OE1	1:A:1138:ARG:NH1	2.40	0.54
2:E:719:TRP:HZ3	2:E:789:MET:HE3	1.72	0.54
2:B:951:LEU:HD21	2:B:986:PHE:HE2	1.73	0.54
2:B:945:LEU:HD22	2:B:972:MET:HE2	1.88	0.54
2:B:857:HIS:O	2:B:918:ASP:OD1	2.25	0.54
1:A:1002:GLU:HG3	1:A:1036:MET:HE3	1.90	0.54
2:E:722:ARG:HB3	2:E:793:VAL:HG12	1.88	0.54
1:G:31:LEU:HD13	1:G:317:LEU:HD21	1.89	0.54
1:G:1061:VAL:HG11	1:G:1104:LYS:HB3	1.88	0.54
1:A:227:GLY:O	1:A:239:TYR:OH	2.26	0.54
3:C:76:ILE:CD1	3:C:198:SER:HB3	2.37	0.54
2:B:732:ILE:HD11	2:B:740:GLN:HG2	1.90	0.53
1:G:184:ASP:HB2	1:G:185:PRO:CD	2.38	0.53
1:G:368:GLU:O	1:G:370:GLN:N	2.37	0.53
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.38	0.53
1:G:7:VAL:HG12	1:G:1091:GLY:HA3	1.90	0.53
2:B:715:THR:O	2:B:716:GLU:HB2	2.07	0.53
1:G:288:GLU:HB2	1:G:298:LYS:HE2	1.89	0.53
2:B:738:TYR:OH	2:B:774:GLU:OE1	2.13	0.53
2:E:917:ILE:HG13	2:E:918:ASP:N	2.24	0.53
1:G:819:CYS:HB2	1:G:875:GLU:HG3	1.92	0.52
2:H:856:LEU:HD11	2:H:915:PRO:HG3	1.91	0.52
1:D:248:ILE:HG12	1:D:250:PRO:HD3	1.91	0.52
3:C:57:ILE:HD11	3:C:96:GLY:HA2	1.92	0.52
2:E:856:LEU:HD13	2:E:884:TYR:HB2	1.91	0.51
2:H:917:ILE:HG13	2:H:918:ASP:N	2.25	0.51
1:G:248:ILE:HG21	1:G:300:LEU:HB2	1.91	0.51
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.46	0.51
2:B:866:LEU:HD11	2:B:876:ALA:HB2	1.92	0.51
1:A:378:CYS:SG	1:A:724:ILE:HB	2.50	0.51
2:B:841:LYS:HD2	2:B:1023:VAL:HB	1.92	0.51
2:B:1035:HIS:CG	2:B:1036:TRP:N	2.75	0.51
1:A:360:VAL:HG11	1:A:721:PRO:O	2.10	0.51
2:E:993:ALA:HB2	2:E:1019:PHE:CE1	2.46	0.51
3:F:243:PRO:HG2	3:F:246:VAL:HG23	1.92	0.51
1:D:43:VAL:HG23	1:D:52:VAL:HG11	1.93	0.50
1:G:1047:TRP:CZ3	1:G:1132:VAL:HG13	2.41	0.50
1:D:324:VAL:HB	1:D:332:GLN:HB2	1.92	0.50
1:D:993:GLN:O	1:D:995:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:794:ILE:HG22	1:D:799:PHE:HA	1.94	0.50
1:D:7:VAL:HG12	1:D:1091:GLY:HA3	1.94	0.49
1:A:926:LEU:HD11	2:B:1038:ASP:HB3	1.93	0.49
3:C:63:ARG:HG3	3:C:123:LEU:HD11	1.94	0.49
1:D:816:LEU:HD13	1:D:831:VAL:HG22	1.94	0.49
1:G:324:VAL:HB	1:G:332:GLN:HG3	1.93	0.49
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.48	0.49
1:D:768:SER:HB3	1:D:847:ARG:NH1	2.28	0.49
2:E:883:LEU:HG	2:E:884:TYR:N	2.27	0.49
2:H:903:PRO:HG2	2:H:906:LEU:HG	1.95	0.49
1:A:6:VAL:HG22	1:A:1040:VAL:HG22	1.95	0.49
1:G:42:TYR:HD1	1:G:51:PRO:HA	1.78	0.49
1:G:317:LEU:HB2	1:G:321:VAL:HG22	1.94	0.49
2:H:842:GLN:CG	2:H:1025:LEU:HD11	2.43	0.49
1:A:1098:LEU:HD22	1:A:1130:ILE:HG23	1.93	0.49
2:E:841:LYS:HG2	2:E:1025:LEU:HD11	1.95	0.49
1:G:949:PHE:CZ	2:H:732:ILE:HG12	2.48	0.49
2:H:737:THR:HG23	2:H:880:LEU:HG	1.95	0.49
2:E:787:VAL:HG23	2:E:874:LYS:HB3	1.95	0.49
3:F:25:TYR:HA	3:F:199:LEU:O	2.12	0.48
2:H:1035:HIS:CG	2:H:1036:TRP:N	2.81	0.48
2:E:936:PHE:CZ	2:E:951:LEU:HD23	2.48	0.48
1:G:190:VAL:O	1:G:209:GLN:HA	2.13	0.48
1:A:1076:PHE:O	1:A:1082:THR:HA	2.13	0.48
1:D:60:LYS:O	1:D:81:THR:HA	2.13	0.48
2:E:844:MET:HE2	2:E:844:MET:HA	1.95	0.48
1:G:1114:TYR:CG	1:G:1124:ALA:HB2	2.49	0.48
2:B:956:CYS:SG	2:B:957:PRO:HD2	2.54	0.48
1:G:59:GLY:HA2	1:G:1073:TRP:CE3	2.48	0.48
1:G:378:CYS:SG	1:G:724:ILE:HB	2.54	0.48
1:A:289:GLU:HG2	1:A:295:VAL:HG22	1.95	0.48
1:D:286:GLU:O	1:D:297:LEU:HD12	2.13	0.48
2:E:931:THR:O	2:E:932:LYS:HB2	2.14	0.48
2:H:793:VAL:HG23	2:H:810:TYR:HB2	1.96	0.48
1:G:63:VAL:O	1:G:79:ILE:HA	2.14	0.48
2:B:823:LEU:HD12	2:B:867:LEU:HD21	1.96	0.47
1:G:143:ILE:HG12	1:G:154:ALA:HB2	1.96	0.47
1:G:998:PHE:CZ	1:G:1074:ARG:HD2	2.49	0.47
2:H:858:ARG:HG2	2:H:917:ILE:HD11	1.96	0.47
1:A:228:GLY:HA3	1:A:241:ASN:HB2	1.96	0.47
1:D:765:VAL:HG22	1:D:806:GLN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:GLN:HG3	1:D:391:ARG:HB3	1.95	0.47
1:D:768:SER:CB	1:D:847:ARG:NH1	2.77	0.47
1:A:63:VAL:O	1:A:79:ILE:HA	2.14	0.47
1:A:170:LEU:HD21	1:A:229:ALA:HB2	1.97	0.47
1:A:226:PHE:HZ	1:A:287:LYS:HG2	1.80	0.47
2:E:897:ILE:HD13	2:E:903:PRO:HD3	1.96	0.47
2:H:1027:LYS:HE2	2:H:1029:ALA:HB2	1.96	0.47
3:I:25:TYR:HA	3:I:199:LEU:O	2.15	0.47
1:A:843:PRO:HG2	1:A:869:ALA:HB2	1.96	0.47
1:A:843:PRO:HG3	2:B:1036:TRP:HH2	1.80	0.47
2:B:835:HIS:HD2	2:B:1029:ALA:CB	2.24	0.47
1:A:1109:VAL:HG21	1:A:1126:ALA:HB2	1.97	0.47
1:G:302:VAL:O	1:G:302:VAL:HG23	2.15	0.47
1:G:790:ASN:HA	1:G:805:HIS:O	2.15	0.47
1:A:725:CYS:SG	1:A:816:LEU:HG	2.54	0.46
1:A:1039:LEU:C	1:A:1039:LEU:HD23	2.39	0.46
2:B:803:LYS:HA	3:C:142:VAL:HG11	1.96	0.46
3:C:25:TYR:HA	3:C:199:LEU:O	2.15	0.46
2:E:953:GLY:O	2:E:1003:LEU:HD11	2.15	0.46
3:F:61:GLY:HA3	3:F:71:LEU:CD2	2.45	0.46
1:G:993:GLN:OE1	1:G:993:GLN:HA	2.15	0.46
1:D:5:TYR:CE2	1:D:7:VAL:HG13	2.51	0.46
2:B:713:ARG:O	2:B:717:SER:OG	2.29	0.46
2:B:787:VAL:HB	2:B:875:LEU:O	2.15	0.46
1:D:146:ASP:OD1	1:D:147:ARG:N	2.49	0.46
1:G:772:SER:OG	1:G:773:SER:N	2.49	0.46
2:H:982:LEU:HD23	2:H:982:LEU:C	2.41	0.46
1:A:358:PRO:O	1:A:379:SER:HA	2.16	0.46
2:E:842:GLN:NE2	2:E:1028:MET:HE1	2.31	0.46
2:H:765:GLU:HA	2:H:765:GLU:OE1	2.15	0.46
2:B:896:VAL:HG13	2:B:897:ILE:HG12	1.98	0.46
1:G:5:TYR:CE2	1:G:7:VAL:HG13	2.51	0.46
1:G:59:GLY:HA2	1:G:1073:TRP:CZ3	2.51	0.46
1:G:220:ILE:O	1:G:229:ALA:HA	2.16	0.46
1:G:289:GLU:HG3	1:G:292:ASP:HA	1.97	0.46
1:D:213:GLU:OE2	1:D:234:GLN:N	2.40	0.46
1:G:330:ASP:HA	1:G:355:ASN:HB3	1.98	0.46
1:D:134:ARG:C	1:D:134:ARG:HD2	2.41	0.46
2:E:737:THR:HG23	2:E:880:LEU:HG	1.98	0.46
1:G:265:ASP:HB3	1:G:267:ASN:OD1	2.16	0.46
1:A:843:PRO:HG3	2:B:1036:TRP:CH2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:816:LEU:HD13	1:G:831:VAL:HG22	1.98	0.46
1:A:791:LEU:HD23	1:A:858:LEU:HD21	1.98	0.45
2:E:763:GLU:HA	2:E:763:GLU:OE1	2.16	0.45
3:F:76:ILE:HD12	3:F:159:HIS:CE1	2.51	0.45
1:G:170:LEU:HD11	1:G:229:ALA:HB2	1.98	0.45
1:A:1117:GLY:O	1:A:1118:SER:HB3	2.17	0.45
1:D:227:GLY:O	1:D:239:TYR:OH	2.34	0.45
2:E:733:ILE:HG21	2:E:743:LYS:HB2	1.96	0.45
1:A:947:ARG:HB3	1:A:949:PHE:CE1	2.52	0.45
2:E:775:ILE:O	2:E:779:ARG:HB2	2.15	0.45
2:E:842:GLN:HE22	2:E:1028:MET:HE1	1.81	0.45
2:B:975:LYS:HE2	2:B:976:LYS:HE3	1.98	0.45
2:B:1010:THR:O	2:B:1014:THR:HG23	2.16	0.45
1:D:849:VAL:HG11	1:D:851:PHE:CZ	2.51	0.45
2:E:872:GLN:N	2:E:1028:MET:HE2	2.31	0.45
1:G:986:ASP:OD1	1:G:986:ASP:N	2.47	0.45
2:B:818:HIS:ND1	2:B:823:LEU:HD21	2.32	0.45
1:G:90:GLU:HB2	1:G:103:ARG:HD2	1.98	0.45
2:H:856:LEU:O	2:H:881:ALA:HA	2.17	0.45
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.52	0.45
1:D:921:ILE:N	1:D:933:LEU:O	2.41	0.45
1:G:246:LEU:HD12	1:G:246:LEU:HA	1.86	0.45
1:G:975:PHE:HA	1:G:996:GLY:O	2.17	0.45
1:G:1114:TYR:CB	1:G:1124:ALA:HB2	2.47	0.45
1:D:286:GLU:OE2	1:D:301:ARG:NH2	2.51	0.44
1:D:933:LEU:HD22	1:D:942:PHE:HB3	1.99	0.44
2:E:759:ARG:O	2:E:760:LEU:HB3	2.17	0.44
3:I:213:LEU:HB2	3:I:251:CYS:SG	2.57	0.44
1:A:926:LEU:O	1:A:953:TRP:HA	2.17	0.44
1:A:971:ALA:HB3	1:A:973:ASN:HD22	1.82	0.44
1:G:36:ASN:O	1:G:37:THR:OG1	2.28	0.44
2:H:793:VAL:CG2	2:H:810:TYR:HB2	2.47	0.44
2:H:1038:ASP:OD1	2:H:1038:ASP:N	2.50	0.44
1:A:719:GLU:OE1	1:A:755:SER:OG	2.31	0.44
1:D:270:ARG:HG2	1:D:284:LEU:HD23	1.98	0.44
1:D:1126:ALA:O	1:D:1130:ILE:HG13	2.17	0.44
1:A:950:ASN:HB2	1:A:994:GLU:OE2	2.16	0.44
1:G:271:TYR:HB2	1:G:283:LEU:HB3	2.00	0.44
2:H:858:ARG:HG2	2:H:917:ILE:CD1	2.48	0.44
2:E:755:LEU:HA	2:E:811:LEU:O	2.18	0.44
1:G:744:ASP:OD1	1:G:746:SER:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:CYS:C	1:D:145:LEU:HD12	2.43	0.44
1:A:376:VAL:HG13	1:A:389:ILE:HD13	1.99	0.44
1:A:830:ILE:HG22	1:A:873:MET:HE1	1.99	0.44
1:G:965:PHE:O	1:G:976:VAL:HA	2.18	0.44
2:E:719:TRP:CZ3	2:E:789:MET:HE3	2.51	0.44
2:E:733:ILE:CG2	2:E:743:LYS:HB2	2.48	0.44
1:G:1124:ALA:HB1	1:G:1128:ASP:CB	2.47	0.44
1:A:709:LYS:HG2	1:A:710:LEU:N	2.33	0.43
1:D:59:GLY:HA2	1:D:1073:TRP:CZ3	2.53	0.43
1:G:926:LEU:O	1:G:953:TRP:HA	2.18	0.43
1:A:843:PRO:CG	1:A:869:ALA:HB2	2.48	0.43
1:A:874:VAL:HG12	1:A:881:LEU:HB3	2.00	0.43
1:G:851:PHE:HB3	1:G:858:LEU:HD22	1.99	0.43
1:A:1058:LEU:HD21	1:A:1097:PHE:HD1	1.83	0.43
1:A:1105:MET:O	1:A:1109:VAL:HG13	2.18	0.43
3:C:63:ARG:HE	3:C:123:LEU:HD21	1.83	0.43
3:F:26:TRP:CD2	3:F:83:MET:HE2	2.53	0.43
2:B:735:GLU:HG2	2:B:740:GLN:HG3	2.01	0.43
1:G:950:ASN:HA	1:G:951:PRO:HD3	1.92	0.43
1:A:965:PHE:O	1:A:976:VAL:HA	2.18	0.43
1:A:1080:ARG:NH2	2:B:928:GLU:OE2	2.50	0.43
1:D:288:GLU:O	1:D:288:GLU:HG3	2.18	0.43
1:D:828:TYR:CE1	1:D:861:VAL:HG21	2.54	0.43
1:G:134:ARG:C	1:G:134:ARG:HD2	2.44	0.43
2:H:945:LEU:HD22	2:H:972:MET:HE2	2.01	0.43
3:I:266:PRO:O	3:I:267:HIS:C	2.59	0.43
1:D:35:LYS:O	1:D:36:ASN:C	2.60	0.43
1:G:213:GLU:HG2	1:G:215:GLU:H	1.84	0.43
1:A:849:VAL:HG11	1:A:851:PHE:CZ	2.54	0.43
2:B:867:LEU:HB3	2:B:873:ILE:HD13	2.00	0.43
1:D:1028:VAL:O	1:D:1039:LEU:HA	2.19	0.42
1:G:282:MET:O	1:G:302:VAL:HA	2.18	0.42
1:G:773:SER:C	1:G:775:THR:N	2.76	0.42
1:G:773:SER:O	1:G:775:THR:N	2.46	0.42
2:H:1025:LEU:HD12	2:H:1025:LEU:HA	1.87	0.42
1:A:1054:MET:HE3	1:A:1129:LEU:HD13	2.00	0.42
2:B:896:VAL:HG12	2:B:906:LEU:CD2	2.48	0.42
2:E:885:ASN:HB3	2:E:889:SER:HB2	2.00	0.42
2:H:996:LEU:O	2:H:1000:MET:HG3	2.19	0.42
2:E:844:MET:HE1	2:E:922:CYS:SG	2.59	0.42
1:G:58:TYR:HB3	1:G:1073:TRP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:184:MET:HE3	3:I:184:MET:HB2	1.82	0.42
1:A:270:ARG:HG2	1:A:284:LEU:HD23	2.02	0.42
2:E:858:ARG:NH1	2:E:880:LEU:O	2.52	0.42
1:G:921:ILE:CD1	1:G:942:PHE:HE1	2.32	0.42
2:H:1036:TRP:O	2:H:1037:GLN:CB	2.66	0.42
1:D:1097:PHE:O	1:D:1105:MET:HE2	2.20	0.42
1:G:985:THR:HB	1:G:988:GLU:HG3	2.01	0.42
1:A:790:ASN:HA	1:A:805:HIS:O	2.20	0.42
1:D:195:VAL:HG22	1:D:202:PHE:HE1	1.85	0.42
1:D:817:VAL:HG22	1:D:830:ILE:HB	2.01	0.42
1:D:985:THR:HB	1:D:988:GLU:HG3	2.01	0.42
1:A:317:LEU:N	1:A:317:LEU:CD1	2.83	0.42
2:B:759:ARG:HG2	2:B:761:ASP:H	1.84	0.42
1:D:926:LEU:O	1:D:953:TRP:HA	2.20	0.42
1:G:232:ILE:HD13	1:G:237:ILE:HG23	2.02	0.42
1:G:374:GLN:HG2	1:G:391:ARG:HB3	2.02	0.42
1:G:983:ALA:HB1	1:G:988:GLU:OE1	2.19	0.42
2:H:1035:HIS:O	2:H:1036:TRP:C	2.62	0.42
2:E:765:GLU:HA	3:F:101:PHE:HZ	1.84	0.42
1:G:259:VAL:O	1:G:259:VAL:HG22	2.20	0.42
2:H:844:MET:HA	2:H:844:MET:HE2	2.01	0.42
1:A:108:VAL:O	1:A:141:LYS:NZ	2.50	0.42
1:A:143:ILE:HG12	1:A:154:ALA:HB2	2.02	0.42
1:A:230:ILE:HD11	1:A:285:LEU:HD21	2.02	0.42
1:A:877:ASN:ND2	1:A:919:ASP:OD1	2.53	0.42
3:F:249:ASP:O	3:F:253:GLN:HG3	2.20	0.42
1:G:93:GLN:HG3	1:G:98:ILE:HG12	2.01	0.42
1:G:246:LEU:HD23	1:G:297:LEU:HD23	2.02	0.42
2:H:774:GLU:O	2:H:778:LEU:HB2	2.20	0.42
1:A:213:GLU:HG2	1:A:215:GLU:H	1.84	0.41
1:A:771:PHE:CE1	1:A:845:GLN:HB3	2.55	0.41
1:A:886:SER:O	1:A:908:ASN:HB2	2.20	0.41
1:D:1014:MET:HE2	1:D:1014:MET:HB2	1.99	0.41
2:E:715:THR:O	2:E:716:GLU:HB2	2.20	0.41
1:G:58:TYR:HB3	1:G:1073:TRP:CB	2.49	0.41
1:G:188:ARG:C	1:G:212:VAL:HG22	2.44	0.41
1:G:223:PRO:HD2	1:G:268:GLY:HA3	2.01	0.41
2:H:867:LEU:HG	2:H:873:ILE:HD13	2.02	0.41
1:A:364:VAL:HG22	1:A:375:LEU:HD13	2.02	0.41
2:E:875:LEU:HD12	2:E:875:LEU:HA	1.85	0.41
2:E:877:ASP:HA	5:E:1101:RMF:C10	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:897:ILE:HG22	2:E:898:THR:N	2.35	0.41
1:G:1011:SER:OG	1:G:1013:VAL:HG22	2.20	0.41
1:G:1023:PRO:HB3	1:G:1047:TRP:CE2	2.56	0.41
1:A:926:LEU:CD1	2:B:1038:ASP:HB3	2.50	0.41
1:A:963:ASP:O	1:A:978:GLN:HA	2.20	0.41
1:D:983:ALA:O	1:D:984:THR:C	2.61	0.41
1:G:773:SER:O	1:G:774:SER:HB3	2.20	0.41
1:A:1007:PHE:CD1	1:A:1030:PHE:HB3	2.55	0.41
2:E:898:THR:O	2:E:899:LEU:C	2.63	0.41
3:F:38:LEU:O	1:G:752:LEU:HA	2.20	0.41
1:G:329:GLY:HA3	1:G:384:GLU:HB3	2.02	0.41
2:H:1036:TRP:O	2:H:1037:GLN:HB2	2.19	0.41
3:I:265:MET:H	3:I:265:MET:HG2	1.68	0.41
1:A:5:TYR:CE2	1:A:7:VAL:HG13	2.56	0.41
1:A:844:LYS:HA	1:A:844:LYS:HD3	1.81	0.41
2:E:887:GLU:H	2:E:887:GLU:CD	2.28	0.41
1:A:32:LEU:HD12	1:A:32:LEU:N	2.36	0.41
1:A:816:LEU:HD13	1:A:831:VAL:HG22	2.03	0.41
1:D:170:LEU:HD11	1:D:179:CYS:HB2	2.02	0.41
3:I:49:TYR:CG	3:I:92:ARG:HD3	2.54	0.41
3:C:76:ILE:HD12	3:C:198:SER:HB3	2.01	0.41
1:D:389:ILE:HD12	1:D:389:ILE:N	2.36	0.41
1:G:770:LEU:HD21	1:G:865:GLU:HB2	2.03	0.41
1:A:7:VAL:CG1	1:A:1091:GLY:HA3	2.50	0.41
1:D:775:THR:HG21	1:D:837:TYR:CE2	2.56	0.41
1:G:368:GLU:HB2	1:G:370:GLN:HG3	2.00	0.41
1:G:980:ASP:HB2	1:G:988:GLU:O	2.21	0.41
1:G:1125:THR:O	1:G:1128:ASP:HB2	2.21	0.41
1:A:387:LEU:HG	1:A:717:LEU:HD11	2.03	0.41
1:A:1028:VAL:O	1:A:1039:LEU:HA	2.21	0.41
1:A:1112:LEU:HD23	1:A:1129:LEU:HD11	2.03	0.41
3:C:125:ASN:OD1	3:C:125:ASN:C	2.64	0.41
1:D:32:LEU:HD12	1:D:32:LEU:N	2.36	0.41
2:E:761:ASP:OD1	2:E:761:ASP:C	2.63	0.41
3:F:264:GLN:HG2	3:F:265:MET:N	2.36	0.41
3:C:266:PRO:O	3:C:267:HIS:C	2.64	0.41
3:C:31:LEU:O	3:C:34:THR:HG23	2.21	0.40
3:C:262:LYS:HA	3:C:262:LYS:HD2	1.85	0.40
2:B:799:ALA:O	2:B:800:LEU:HB2	2.21	0.40
1:D:986:ASP:O	1:D:990:GLN:HG3	2.21	0.40
1:D:1030:PHE:CZ	1:D:1038:GLY:HA3	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:266:PRO:O	3:F:267:HIS:C	2.63	0.40
1:G:14:ALA:O	1:G:35:LYS:HG2	2.21	0.40
1:G:909:ILE:HD13	1:G:909:ILE:HA	1.89	0.40
1:G:1030:PHE:CZ	1:G:1038:GLY:HA3	2.56	0.40
1:A:64:MET:HG3	1:A:77:LEU:HD11	2.03	0.40
2:B:766:GLY:N	3:C:141:MET:HE1	2.36	0.40
2:B:778:LEU:HD21	2:B:878:PHE:CD2	2.56	0.40
1:D:1105:MET:SD	1:D:1130:ILE:HD11	2.62	0.40
1:D:790:ASN:HA	1:D:805:HIS:O	2.20	0.40
1:G:170:LEU:HD12	1:G:170:LEU:HA	1.89	0.40
2:H:760:LEU:HD12	2:H:760:LEU:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:GLU:O	2:H:888:GLU:OE2[4_565]	2.15	0.05
2:E:1018:ASP:OD2	3:I:232:ARG:HE[5_554]	1.59	0.01

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	822/840 (98%)	798 (97%)	22 (3%)	2 (0%)	43	70
1	D	823/840 (98%)	805 (98%)	17 (2%)	1 (0%)	48	76
1	G	822/840 (98%)	799 (97%)	23 (3%)	0	100	100
2	B	329/344 (96%)	321 (98%)	8 (2%)	0	100	100
2	E	328/344 (95%)	316 (96%)	12 (4%)	0	100	100
2	H	328/344 (95%)	317 (97%)	10 (3%)	1 (0%)	36	64
3	C	246/271 (91%)	242 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	246/271 (91%)	242 (98%)	4 (2%)	0	100	100
3	I	246/271 (91%)	242 (98%)	4 (2%)	0	100	100
All	All	4190/4365 (96%)	4082 (97%)	104 (2%)	4 (0%)	48	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	369	ARG
2	H	1037	GLN
1	A	772	SER
1	A	981	SER

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	721/728 (99%)	707 (98%)	14 (2%)	50	69
1	D	722/728 (99%)	719 (100%)	3 (0%)	84	84
1	G	721/728 (99%)	708 (98%)	13 (2%)	51	69
2	B	299/308 (97%)	288 (96%)	11 (4%)	30	57
2	E	298/308 (97%)	284 (95%)	14 (5%)	23	51
2	H	298/308 (97%)	289 (97%)	9 (3%)	36	61
3	C	223/242 (92%)	222 (100%)	1 (0%)	84	84
3	F	223/242 (92%)	222 (100%)	1 (0%)	84	84
3	I	223/242 (92%)	222 (100%)	1 (0%)	84	84
All	All	3728/3834 (97%)	3661 (98%)	67 (2%)	51	69

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ILE
1	A	258	ILE

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Mol	Chain	Res	Type
1	A	259	VAL
1	A	260	CYS
1	A	284	LEU
1	A	302	VAL
1	A	307	GLU
1	A	317	LEU
1	A	766	SER
1	A	870	VAL
1	A	993	GLN
1	A	1020	THR
1	A	1116	ASP
1	A	1127	ASP
2	B	755	LEU
2	B	787	VAL
2	B	863	SER
2	B	866	LEU
2	B	867	LEU
2	B	888	GLU
2	B	896	VAL
2	B	897	ILE
2	B	964	ILE
2	B	1036	TRP
2	B	1040	HIS
3	C	257	LEU
1	D	209	GLN
1	D	766	SER
1	D	794	ILE
2	E	755	LEU
2	E	761	ASP
2	E	765	GLU
2	E	797	GLN
2	E	863	SER
2	E	873	ILE
2	E	882	ARG
2	E	886	SER
2	E	887	GLU
2	E	906	LEU
2	E	1036	TRP
2	E	1038	ASP
2	E	1040	HIS
2	E	1042	LEU
3	F	142	VAL

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Mol	Chain	Res	Type
1	G	20	THR
1	G	52	VAL
1	G	74	LYS
1	G	258	ILE
1	G	294	THR
1	G	321	VAL
1	G	360	VAL
1	G	720	SER
1	G	781	SER
1	G	794	ILE
1	G	1113	GLN
1	G	1120	MET
1	G	1123	GLU
2	H	787	VAL
2	H	844	MET
2	H	852	LYS
2	H	863	SER
2	H	897	ILE
2	H	940	LEU
2	H	1025	LEU
2	H	1033	LEU
2	H	1035	HIS
3	I	144	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	790	ASN
1	A	970	ASN
1	A	978	GLN
1	A	991	HIS
1	A	993	GLN
2	B	835	HIS
2	B	944	GLN
3	C	156	GLN
3	C	267	HIS
1	D	16	ASN
1	D	211	ASN
1	D	290	GLN
1	D	372	GLN
1	D	964	ASN

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Mol	Chain	Res	Type
1	D	978	GLN
2	E	851	HIS
2	E	977	GLN
3	F	179	GLN
1	G	240	HIS
1	G	731	GLN
1	G	826	ASN
1	G	908	ASN
1	G	991	HIS
1	G	1015	GLN
2	H	894	ASN
2	H	977	GLN
2	H	999	HIS
2	H	1040	HIS
3	I	37	GLN
3	I	252	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TPO	B	893	2	8,10,11	1.96	3 (37%)	10,14,16	1.48	2 (20%)
2	TPO	H	893	2	8,10,11	1.91	3 (37%)	10,14,16	1.64	1 (10%)
2	TPO	E	893	2	8,10,11	1.99	3 (37%)	10,14,16	1.26	1 (10%)

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
2	TPO	B	893	2	-	1/9/11/13	-
2	TPO	H	893	2	-	0/9/11/13	-
2	TPO	E	893	2	-	0/9/11/13	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	893	TPO	P-O1P	3.91	1.62	1.50
2	H	893	TPO	P-OG1	3.87	1.66	1.59
2	B	893	TPO	P-O1P	3.87	1.62	1.50
2	E	893	TPO	P-OG1	2.76	1.64	1.59
2	H	893	TPO	P-O3P	2.30	1.63	1.54
2	B	893	TPO	P-OG1	2.29	1.63	1.59
2	B	893	TPO	P-O2P	2.13	1.62	1.54
2	E	893	TPO	P-O3P	2.03	1.62	1.54
2	H	893	TPO	P-O2P	2.01	1.62	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	893	TPO	CG2-CB-CA	-3.91	105.65	113.26
2	E	893	TPO	CG2-CB-CA	-2.41	108.56	113.26
2	B	893	TPO	O2P-P-OG1	2.30	114.79	105.85
2	B	893	TPO	CG2-CB-CA	-2.27	108.84	113.26

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	893	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

9 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
5	RMF	E	1101	-	39,39,39	0.57	0	49,57,57	1.59	4 (8%)
4	SO4	H	1102	-	4,4,4	0.38	0	6,6,6	0.07	0
6	CIT	I	301	-	12,12,12	1.75	4 (33%)	17,17,17	1.98	7 (41%)
6	CIT	C	301	-	12,12,12	1.27	0	17,17,17	2.25	9 (52%)
6	CIT	F	301	-	12,12,12	1.43	2 (16%)	17,17,17	1.75	5 (29%)
5	RMF	H	1101	-	39,39,39	0.54	0	49,57,57	1.60	5 (10%)
4	SO4	G	1201	-	4,4,4	0.44	0	6,6,6	0.12	0
4	SO4	A	1201	-	4,4,4	0.45	0	6,6,6	0.11	0
5	RMF	B	1101	-	39,39,39	0.55	0	49,57,57	1.60	5 (10%)

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	RMF	E	1101	-	-	3/12/21/21	0/6/6/6
6	CIT	C	301	-	-	0/16/16/16	-
6	CIT	F	301	-	-	4/16/16/16	-
5	RMF	H	1101	-	-	5/12/21/21	0/6/6/6
6	CIT	I	301	-	-	12/16/16/16	-
5	RMF	B	1101	-	-	3/12/21/21	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	301	CIT	C2-C3	-3.48	1.49	1.54
6	I	301	CIT	C4-C3	-2.83	1.50	1.54
6	F	301	CIT	C2-C3	-2.16	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	301	CIT	O1-C1	2.11	1.29	1.22
6	I	301	CIT	O3-C5	2.04	1.28	1.22
6	F	301	CIT	O3-C5	2.03	1.28	1.22

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1101	RMF	C14-N6-C3	-5.86	110.09	121.67
5	B	1101	RMF	C11-N6-C3	-5.62	110.56	121.67
5	H	1101	RMF	C11-N6-C3	-5.53	110.74	121.67
5	E	1101	RMF	C14-N6-C3	-5.49	110.82	121.67
5	E	1101	RMF	C11-N6-C3	-5.25	111.28	121.67
5	H	1101	RMF	C14-N6-C3	-4.92	111.95	121.67
5	E	1101	RMF	C4-N5-C6	4.62	107.50	105.35
6	F	301	CIT	O6-C6-C3	4.51	121.80	113.14
5	E	1101	RMF	N5-C6-N4	-4.44	111.35	113.88
5	H	1101	RMF	C4-N5-C6	4.31	107.36	105.35
6	I	301	CIT	O6-C6-C3	4.12	121.04	113.14
5	H	1101	RMF	N5-C6-N4	-4.07	111.57	113.88
5	B	1101	RMF	C4-N5-C6	4.06	107.24	105.35
5	B	1101	RMF	N5-C6-N4	-4.04	111.58	113.88
6	C	301	CIT	C2-C3-C6	-3.87	101.48	110.03
6	C	301	CIT	O6-C6-C3	3.30	119.46	113.14
6	C	301	CIT	O7-C3-C6	3.26	113.59	108.96
6	I	301	CIT	O4-C5-C4	3.00	123.84	114.35
6	I	301	CIT	O2-C1-C2	2.95	123.70	114.35
6	C	301	CIT	O7-C3-C2	2.90	115.98	109.38
6	I	301	CIT	O2-C1-O1	-2.84	116.04	123.33
6	C	301	CIT	O2-C1-C2	2.73	123.00	114.35
6	F	301	CIT	O2-C1-O1	-2.65	116.50	123.33
6	C	301	CIT	O4-C5-O3	-2.49	116.92	123.33
6	I	301	CIT	O4-C5-O3	-2.49	116.94	123.33
6	C	301	CIT	O2-C1-O1	-2.45	117.04	123.33
6	F	301	CIT	O4-C5-O3	-2.45	117.04	123.33
6	I	301	CIT	O6-C6-O5	-2.35	116.35	123.86
6	F	301	CIT	O4-C5-C4	2.32	121.70	114.35
6	F	301	CIT	O6-C6-O5	-2.30	116.51	123.86
5	H	1101	RMF	C5-C4-N3	-2.23	124.83	127.18
5	B	1101	RMF	C5-C4-N3	-2.22	124.84	127.18
6	C	301	CIT	C4-C3-C6	-2.11	105.36	110.03
6	I	301	CIT	O7-C3-C6	-2.07	106.02	108.96
6	C	301	CIT	O7-C3-C4	2.04	114.03	109.38

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1101	RMF	N2-C3-N6-C14
5	B	1101	RMF	N3-C3-N6-C14
5	E	1101	RMF	N2-C3-N6-C11
5	E	1101	RMF	N3-C3-N6-C11
5	H	1101	RMF	N2-C3-N6-C14
5	H	1101	RMF	N3-C3-N6-C14
6	I	301	CIT	C2-C3-C6-O5
6	I	301	CIT	C2-C3-C6-O6
6	I	301	CIT	O7-C3-C6-O5
6	I	301	CIT	O7-C3-C6-O6
6	I	301	CIT	C1-C2-C3-O7
6	I	301	CIT	O7-C3-C4-C5
6	F	301	CIT	C1-C2-C3-O7
6	F	301	CIT	C1-C2-C3-C6
6	I	301	CIT	C1-C2-C3-C4
6	I	301	CIT	C2-C3-C4-C5
6	I	301	CIT	C6-C3-C4-C5
5	E	1101	RMF	C5-C2-N1-C1
6	I	301	CIT	C4-C3-C6-O5
6	I	301	CIT	C1-C2-C3-C6
5	H	1101	RMF	C9-C7-N5-C6
5	B	1101	RMF	C5-C2-N1-C1
6	I	301	CIT	C4-C3-C6-O6
5	H	1101	RMF	C5-C2-N1-C1
5	H	1101	RMF	N1-C1-C15-N10
6	F	301	CIT	C1-C2-C3-C4
6	F	301	CIT	O7-C3-C4-C5

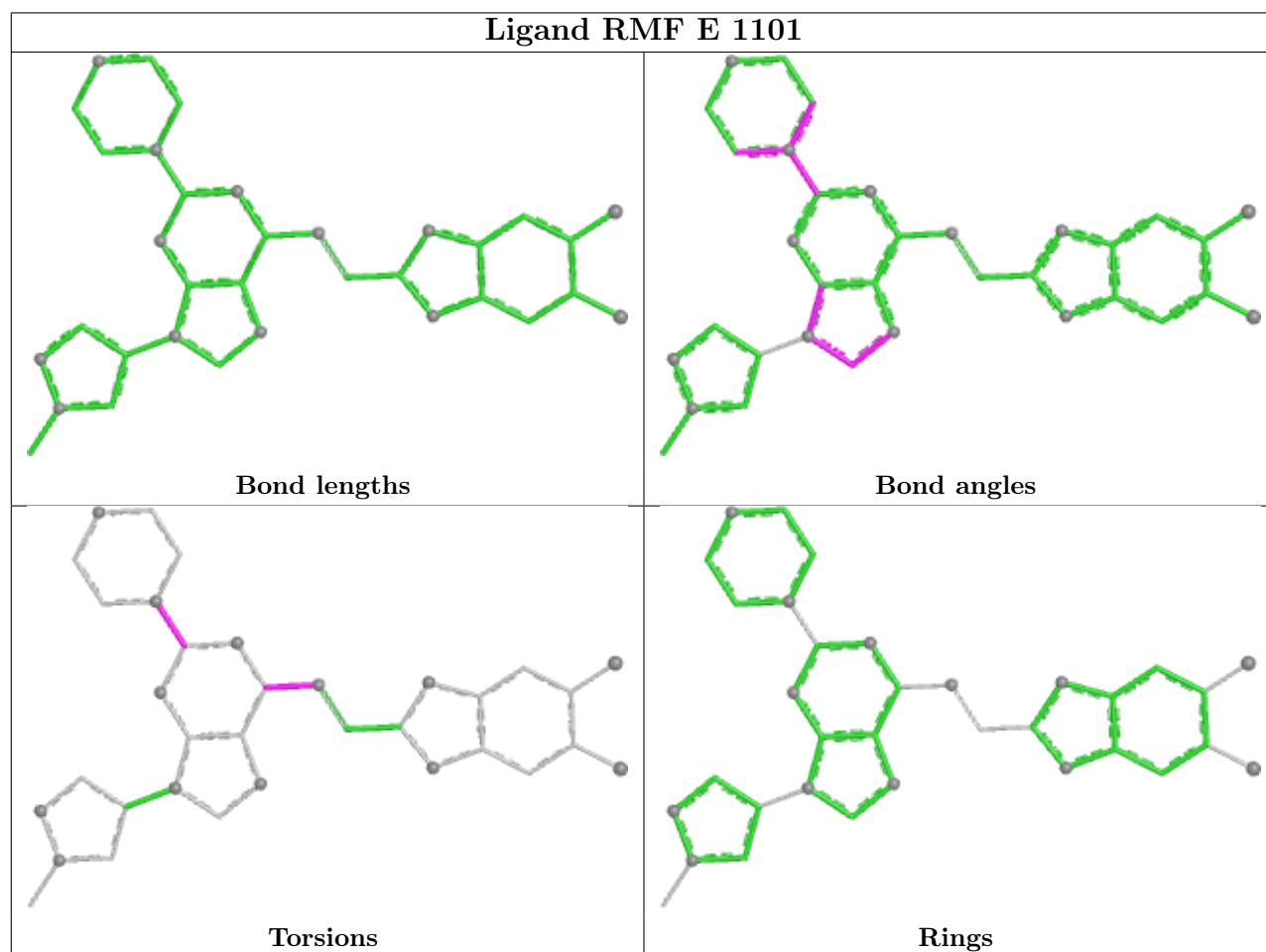
There are no ring outliers.

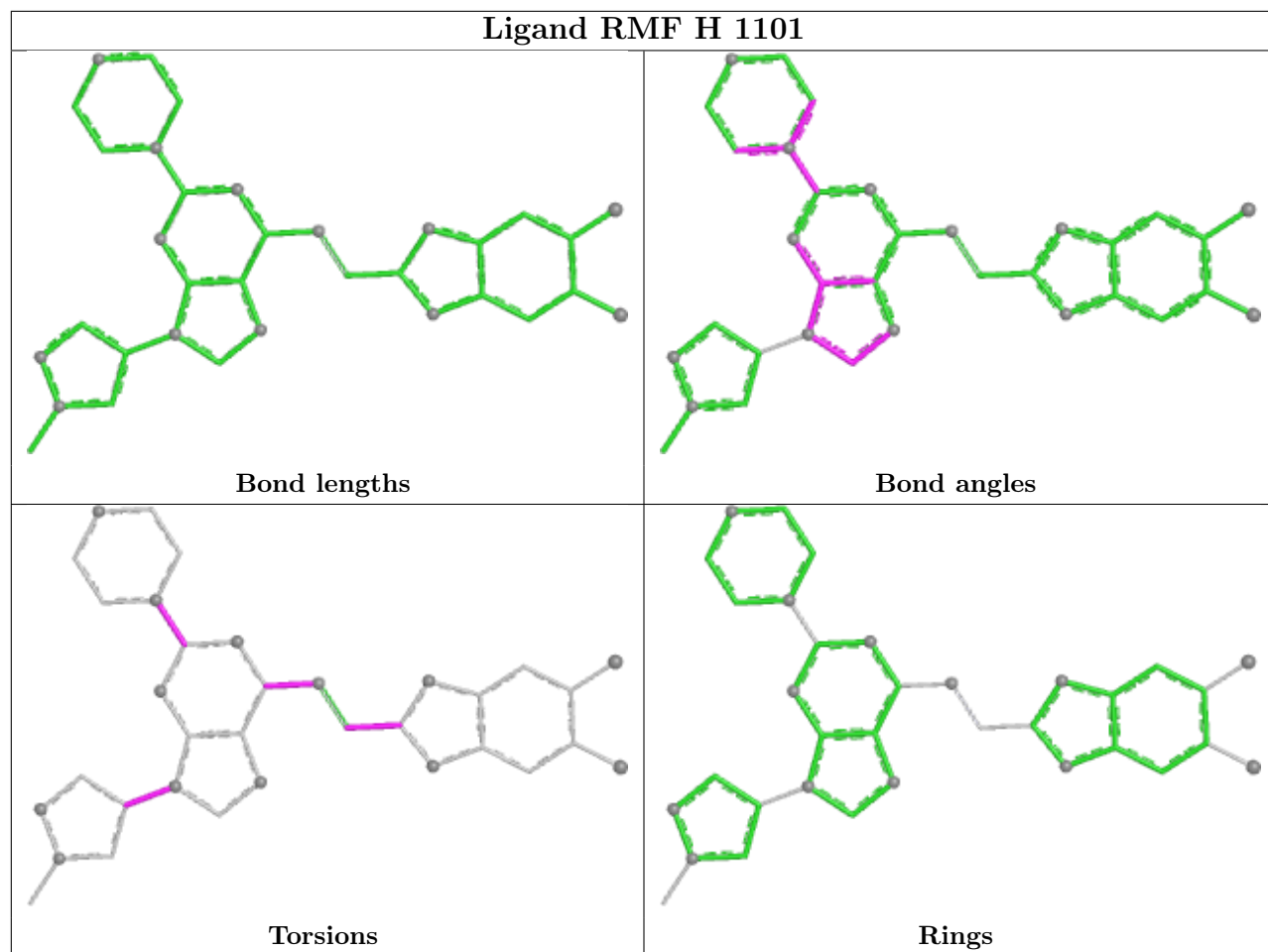
1 monomer is involved in 1 short contact:

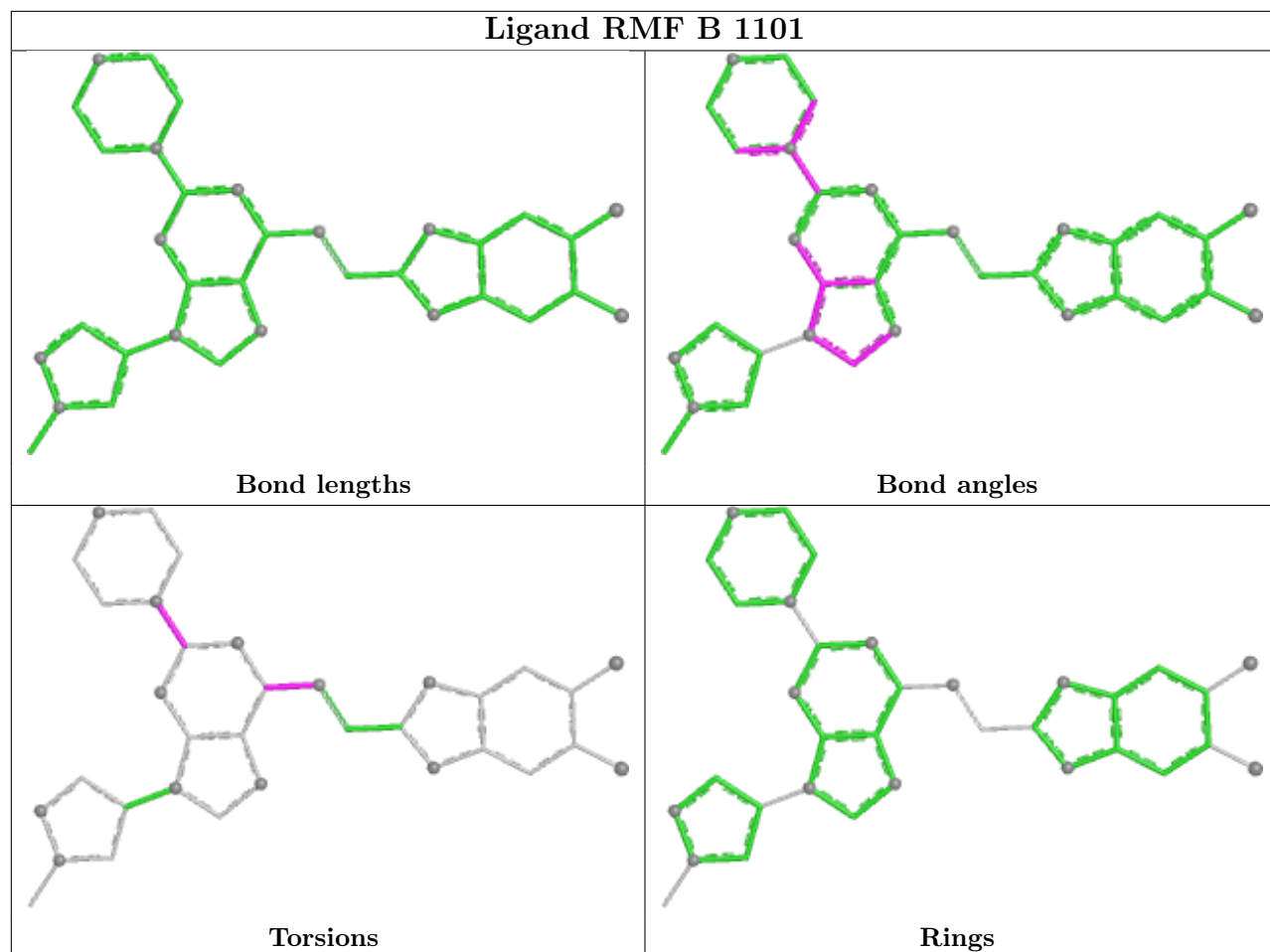
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1101	RMF	1	0

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	821/840 (97%)	-0.41	1 (0%) 92 86	37, 65, 112, 170	0
1	D	827/840 (98%)	-0.45	1 (0%) 92 86	37, 62, 107, 163	0
1	G	826/840 (98%)	-0.26	5 (0%) 85 70	42, 75, 127, 189	0
2	B	331/344 (96%)	-0.31	5 (1%) 72 51	42, 66, 102, 167	0
2	E	330/344 (95%)	-0.30	2 (0%) 85 70	39, 60, 101, 161	0
2	H	330/344 (95%)	-0.28	4 (1%) 76 57	36, 57, 100, 133	0
3	C	248/271 (91%)	-0.58	1 (0%) 88 76	40, 59, 99, 125	0
3	F	248/271 (91%)	-0.63	0 100 100	34, 50, 86, 119	0
3	I	248/271 (91%)	-0.56	0 100 100	36, 54, 90, 136	0
All	All	4209/4365 (96%)	-0.40	19 (0%) 87 73	34, 63, 111, 189	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1042	LEU	4.2
2	B	1042	LEU	3.5
2	H	1043	TRP	3.5
2	E	1043	TRP	3.4
1	D	394	ILE	3.3
2	E	1042	LEU	3.1
2	H	1029	ALA	2.8
2	B	1043	TRP	2.6
1	G	394	ILE	2.5
3	C	20	THR	2.4
2	B	1036	TRP	2.3
1	A	393	GLY	2.3
2	H	800	LEU	2.3
1	G	1050	LEU	2.3
1	G	264	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	317	LEU	2.1
1	G	122	GLY	2.1
2	B	1041	GLU	2.1
2	B	1044	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	TPO	B	893	11/12	0.64	0.13	150,174,202,207	6
2	TPO	H	893	11/12	0.73	0.14	115,127,153,158	6
2	TPO	E	893	11/12	0.79	0.14	145,156,185,187	6

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.

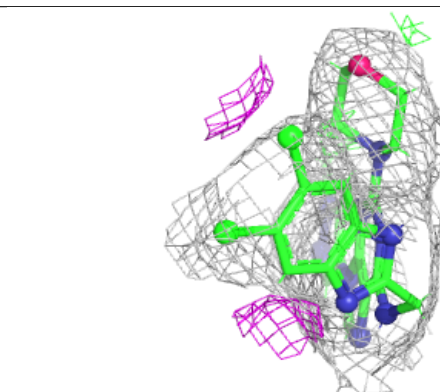
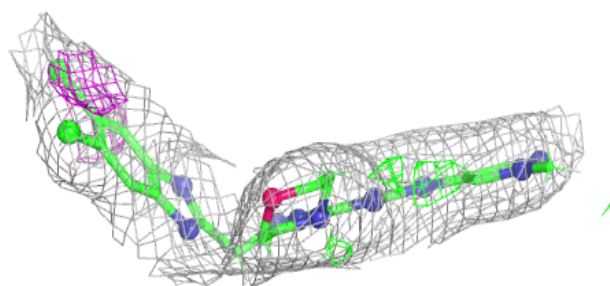
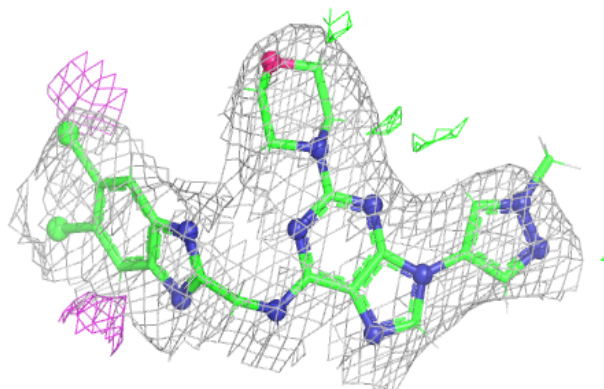
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CIT	I	301	13/13	0.51	0.11	107,114,138,138	5
6	CIT	F	301	13/13	0.67	0.11	101,104,125,125	5
4	SO4	G	1201	5/5	0.68	0.07	171,172,175,234	0
6	CIT	C	301	13/13	0.68	0.09	114,117,140,140	5
4	SO4	H	1102	5/5	0.80	0.08	127,128,135,191	0
4	SO4	A	1201	5/5	0.86	0.05	149,153,163,229	0
5	RMF	E	1101	34/34	0.93	0.10	94,106,131,152	20
5	RMF	H	1101	34/34	0.95	0.09	94,111,138,152	20
5	RMF	B	1101	34/34	0.95	0.08	101,111,136,153	20

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

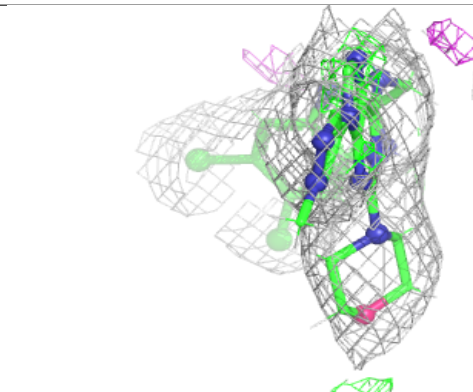
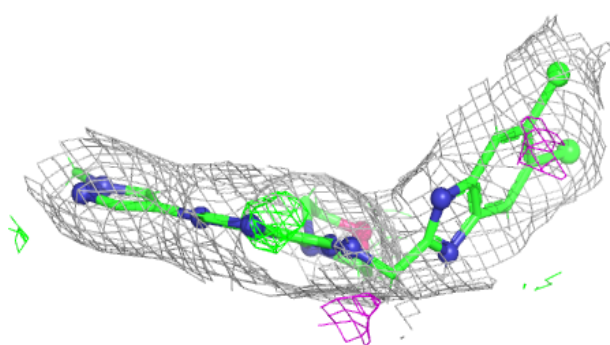
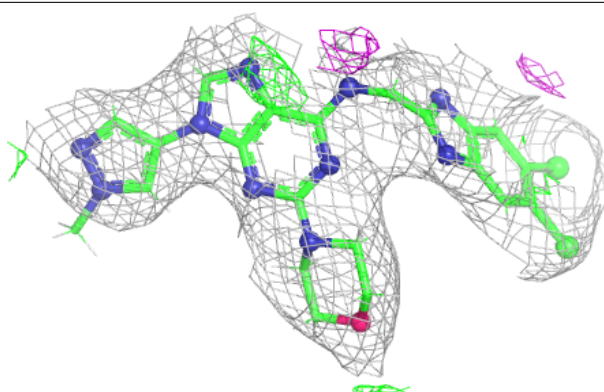
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around RMF E 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

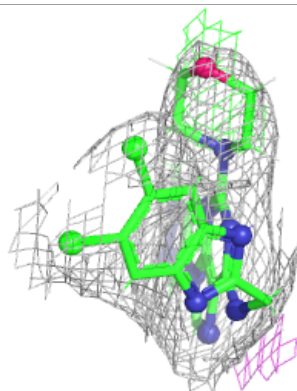
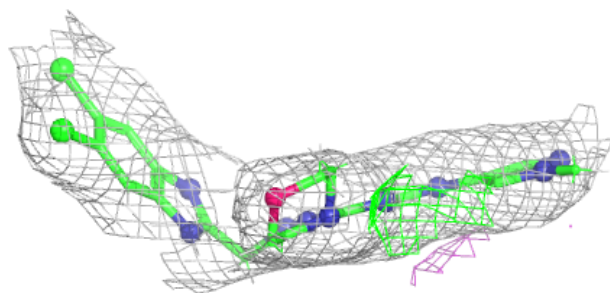
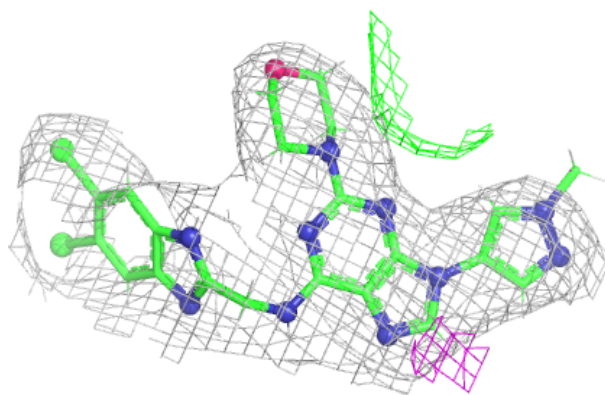
**Electron density around RMF H 1101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around RMF B 1101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.