



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:32 pm GMT

PDB ID : 4DWK
Title : Structure of cystein free insulin degrading enzyme with compound bdm41671 ((s)-2-{2-[carboxymethyl-(3-phenyl-propyl)-amino]-acetyl-amino}-3-(1h-imidazol-4-yl)-propionic acid methyl ester)
Authors : Guo, Q.; Deprez-Poulain, R.; Deprez, B.; Tang, W.J.
Deposited on : 2012-02-24
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk28620

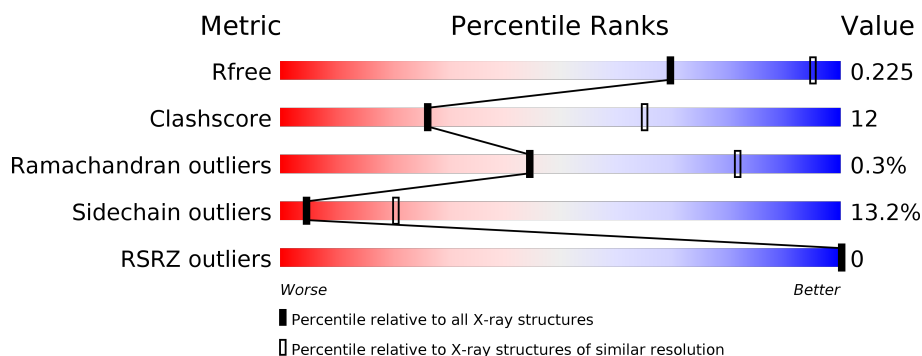
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	990	
1	B	990	

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
2	MGK	A	1101	-	-	-	X
2	MGK	B	1101	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15764 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	955	Total	C	N	O	S	0	0	0
			7802	5026	1310	1443	23			
1	B	955	Total	C	N	O	S	0	0	0
			7796	5023	1309	1442	22			

There are 52 discrepancies between the modelled and reference sequences:

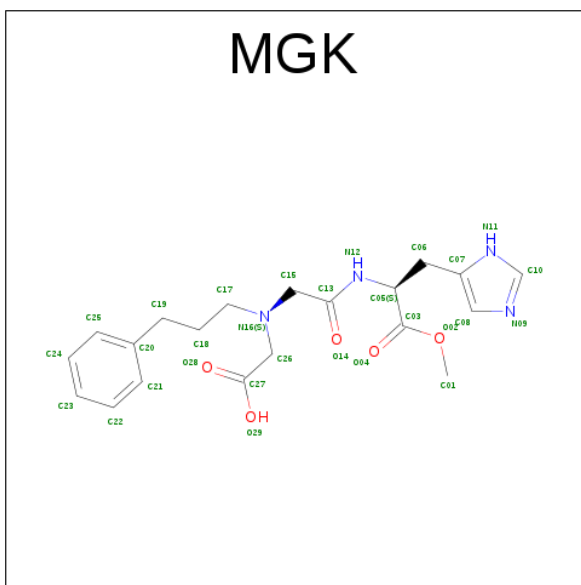
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	EXPRESSION TAG	UNP P14735
A	31	HIS	-	EXPRESSION TAG	UNP P14735
A	32	HIS	-	EXPRESSION TAG	UNP P14735
A	33	HIS	-	EXPRESSION TAG	UNP P14735
A	34	HIS	-	EXPRESSION TAG	UNP P14735
A	35	HIS	-	EXPRESSION TAG	UNP P14735
A	36	HIS	-	EXPRESSION TAG	UNP P14735
A	37	ALA	-	EXPRESSION TAG	UNP P14735
A	38	ALA	-	EXPRESSION TAG	UNP P14735
A	39	GLY	-	EXPRESSION TAG	UNP P14735
A	40	ILE	-	EXPRESSION TAG	UNP P14735
A	41	PRO	-	EXPRESSION TAG	UNP P14735
A	110	LEU	CYS	ENGINEERED MUTATION	UNP P14735
A	111	GLN	GLU	ENGINEERED MUTATION	UNP P14735
A	171	SER	CYS	ENGINEERED MUTATION	UNP P14735
A	178	ALA	CYS	ENGINEERED MUTATION	UNP P14735
A	257	VAL	CYS	ENGINEERED MUTATION	UNP P14735
A	414	LEU	CYS	ENGINEERED MUTATION	UNP P14735
A	573	ASN	CYS	ENGINEERED MUTATION	UNP P14735
A	590	SER	CYS	ENGINEERED MUTATION	UNP P14735
A	789	SER	CYS	ENGINEERED MUTATION	UNP P14735
A	812	ALA	CYS	ENGINEERED MUTATION	UNP P14735
A	819	ALA	CYS	ENGINEERED MUTATION	UNP P14735
A	904	SER	CYS	ENGINEERED MUTATION	UNP P14735
A	966	ASN	CYS	ENGINEERED MUTATION	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
A	974	ALA	CYS	ENGINEERED MUTATION	UNP P14735
B	30	MET	-	EXPRESSION TAG	UNP P14735
B	31	HIS	-	EXPRESSION TAG	UNP P14735
B	32	HIS	-	EXPRESSION TAG	UNP P14735
B	33	HIS	-	EXPRESSION TAG	UNP P14735
B	34	HIS	-	EXPRESSION TAG	UNP P14735
B	35	HIS	-	EXPRESSION TAG	UNP P14735
B	36	HIS	-	EXPRESSION TAG	UNP P14735
B	37	ALA	-	EXPRESSION TAG	UNP P14735
B	38	ALA	-	EXPRESSION TAG	UNP P14735
B	39	GLY	-	EXPRESSION TAG	UNP P14735
B	40	ILE	-	EXPRESSION TAG	UNP P14735
B	41	PRO	-	EXPRESSION TAG	UNP P14735
B	110	LEU	CYS	ENGINEERED MUTATION	UNP P14735
B	111	GLN	GLU	ENGINEERED MUTATION	UNP P14735
B	171	SER	CYS	ENGINEERED MUTATION	UNP P14735
B	178	ALA	CYS	ENGINEERED MUTATION	UNP P14735
B	257	VAL	CYS	ENGINEERED MUTATION	UNP P14735
B	414	LEU	CYS	ENGINEERED MUTATION	UNP P14735
B	573	ASN	CYS	ENGINEERED MUTATION	UNP P14735
B	590	SER	CYS	ENGINEERED MUTATION	UNP P14735
B	789	SER	CYS	ENGINEERED MUTATION	UNP P14735
B	812	ALA	CYS	ENGINEERED MUTATION	UNP P14735
B	819	ALA	CYS	ENGINEERED MUTATION	UNP P14735
B	904	SER	CYS	ENGINEERED MUTATION	UNP P14735
B	966	ASN	CYS	ENGINEERED MUTATION	UNP P14735
B	974	ALA	CYS	ENGINEERED MUTATION	UNP P14735

- Molecule 2 is METHYL N-(CARBOXYMETHYL)-N-(3-PHENYLPROPYL)GLYCYL-L-HISTIDINATE (three-letter code: MGK) (formula: C₂₀H₂₆N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	20	4	5		
2	B	1	Total	C	N	O	0	0
			29	20	4	5		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total	O	0	0
			67	67		
4	B	39	Total	O	0	0
			39	39		

ILE	N979	L980	E990	Q993	N994	E997	F998	K999	L1002	P1003	L1007	V1008	K1009	P1010	H1011	ILE	ASN	PHE	MET	ALA	ALA	LYS	LEU																								
A888	L889	A890	I891	R892	R893	K898	K899	S904	I912	Q915	R920	T923	E924	Y927	L928	T932	K933	E934	D935	Y940	K941	E942	A945	V946	D947	A948	R951	H952	K953	V956	H957	E962	S965	ASN	PRO	VAL	VAL	GLY	GLU	PHE	PRO	ALA	GLN	ASN	ASP		
S803	E804	N805	M806	R807	L808	E809	L810	I815	S816	E817	P818	L823	K826	E827	Y831	R838	R839	A840	N841	G842	I843	Q844	G845	L846	R847	S852	E853	K854	P855	P856	L859	E860	S861	R862	A865	F866	L867	I868	T869	M870	I874	M877	E880	K884	H885	I886	Q887
E702	T708	L709	P710	R711	L712	K713	Q718	I725	L728	L729	H730	I733	T734	K735	Q736	M742	Q743	A840	N841	G842	I843	Q844	G845	L846	R847	S852	E853	K854	P855	P856	L859	E860	S861	R862	A865	F866	L867	I868	T869	M870	I874	M877	E880	K884	H885	I886	Q887
E598	L599	L600	K601	D602	S603	L604	R605	E606	E612	L616	N622	G626	M627	V628	L629	S630	V631	Q638	L642	K643	K644	E647	K648	D655	E656	K657	R658	F659	T662	K663	E664	N671	N672	F673	R674	A675	E676	Q677	Y685	L686	T691	E692	V693	A694	W695	K701	
E465	D469	S475	N476	V481	E494	T498	D507	E508	K511	K512	W513	Q514	D517	G520	K521	F522	K523	L524	K527	N528	E529	F535	L538	K552	M556	L559	P570	N576	F576	E577	F578	F579	A583	D586	P587	E458	F459	R460	P461	Y596	L597						
L226	R229	L131	E233	R238	Q239	L242	K243	S250	S251	V256	V257	V258	L259	E262	L270	V271	V272	S276	K281	L285	P286	E287	E290	Q294	H297	L298	I304	K308	D309	I310	R311	T316	F317	P318	N329	P330	G331	H332	L337	E341							
L346	L347	S348	E349	K353	L359	V360	Q363	K364	R368	K371	L379	H386	D389	Q399	E413	L414	L417	K425	Y433	I437	I440	L441	Y444	L445	E447	E448	V449	L450	T451	A452	E453	Y454	L455	L456	E457	E458	F459	R460	P461	Y462							
S128	Q129	F130	L131	E132	E133	H134	S138	E145	H146	T147	N148	Y149	Y150	F151	H157	L158	E159	G160	R164	Q167	L170	D175	E176	S177	A178	K179	N184	S188	E189	V194	M195	N196	D197	A198	W199	R200	L201	F202	Q203	K206	P214	F215	S216	K217	K223		

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	261.51Å 261.51Å 91.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.45 – 3.00 49.42 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.45-3.00) 99.5 (49.42-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.177 , 0.227 0.179 , 0.225	Depositor DCC
R_{free} test set	3623 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15764	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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: MGK, 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	0.93	5/7996 (0.1%)	0.94	12/10817 (0.1%)
1	B	0.91	9/7990 (0.1%)	0.91	10/10810 (0.1%)
All	All	0.92	14/15986 (0.1%)	0.93	22/21627 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	GLU	CG-CD	9.59	1.66	1.51
1	B	189	GLU	CG-CD	8.38	1.64	1.51
1	A	577	GLU	CG-CD	8.11	1.64	1.51
1	A	189	GLU	CB-CG	8.06	1.67	1.52
1	B	189	GLU	CD-OE1	7.16	1.33	1.25
1	B	577	GLU	CG-CD	6.96	1.62	1.51
1	B	287	GLU	CG-CD	6.61	1.61	1.51
1	B	287	GLU	CB-CG	6.04	1.63	1.52
1	B	453	GLU	CB-CG	6.01	1.63	1.52
1	B	189	GLU	CB-CG	5.99	1.63	1.52
1	B	529	GLU	CB-CG	5.67	1.62	1.52
1	A	176	GLU	CG-CD	5.62	1.60	1.51
1	A	880	GLU	CG-CD	5.62	1.60	1.51
1	B	494	GLU	CG-CD	5.01	1.59	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	GLU	OE1-CD-OE2	-13.54	107.06	123.30
1	A	50	ILE	CB-CA-C	-7.93	95.74	111.60
1	B	847	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	B	674	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	189	GLU	CG-CD-OE2	6.75	131.81	118.30
1	A	226	LEU	CA-CB-CG	6.22	129.61	115.30
1	A	67	LEU	CA-CB-CG	6.21	129.58	115.30
1	A	253	LEU	CB-CG-CD1	-6.19	100.47	111.00
1	B	189	GLU	CA-CB-CG	5.98	126.56	113.40
1	A	285	LEU	CA-CB-CG	5.76	128.56	115.30
1	B	456	LEU	CB-CA-C	-5.75	99.27	110.20
1	A	892	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	B	189	GLU	N-CA-CB	5.61	120.70	110.60
1	B	49	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	97	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	92	VAL	CB-CA-C	-5.25	101.44	111.40
1	B	175	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	243	LYS	CD-CE-NZ	5.22	123.71	111.70
1	A	170	LEU	CA-CB-CG	-5.13	103.49	115.30
1	A	189	GLU	CA-CB-CG	5.10	124.62	113.40
1	A	626	GLY	N-CA-C	-5.05	100.48	113.10
1	B	771	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	979	ASN	Peptide
1	B	455	LEU	Peptide
1	B	979	ASN	Peptide

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	7802	0	7740	172	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7796	0	7729	192	0
2	A	29	0	25	2	0
2	B	29	0	25	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	67	0	0	3	0
4	B	39	0	0	3	0
All	All	15764	0	15519	366	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 12.

All (366) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLU:HG2	1:B:347:LEU:HD12	1.34	1.05
1:B:774:ARG:HG3	1:B:774:ARG:HH11	1.24	1.00
1:A:50:ILE:O	1:A:50:ILE:HG22	1.61	0.99
1:A:622:ASN:H	1:A:622:ASN:HD22	1.03	0.96
1:A:622:ASN:H	1:A:622:ASN:ND2	1.62	0.95
1:A:491:ARG:HG3	1:A:491:ARG:HH11	1.33	0.94
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.52	0.91
1:B:754:HIS:CE1	4:B:1236:HOH:O	2.28	0.85
1:B:622:ASN:H	1:B:622:ASN:HD22	1.25	0.84
1:B:348:SER:OG	1:B:606:GLU:OE2	1.97	0.81
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.62	0.80
1:B:754:HIS:HE1	4:B:1236:HOH:O	1.62	0.79
1:A:294:GLN:H	1:A:297:HIS:HD2	1.31	0.77
2:B:1101:MGK:H26A	2:B:1101:MGK:O14	1.84	0.76
1:A:722:ARG:HB2	1:A:758:LEU:HD12	1.67	0.76
1:B:206:LYS:HG2	1:B:215:PHE:O	1.85	0.76
1:A:722:ARG:HB2	1:A:758:LEU:CD1	2.16	0.75
1:B:189:GLU:HG2	1:B:831:TYR:CE1	2.22	0.75
1:A:309:ASP:H	1:A:672:ASN:HD21	1.32	0.75
1:A:491:ARG:NH1	1:A:491:ARG:HG3	1.96	0.75
1:B:774:ARG:CG	1:B:774:ARG:HH11	1.99	0.75
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.87	0.74
1:B:827:GLU:OE1	1:B:862:ARG:HD3	1.86	0.74
1:A:730:HIS:HD2	1:A:904:SER:OG	1.71	0.73
1:A:927:TYR:O	1:A:930:THR:HB	1.86	0.73
1:A:50:ILE:O	1:A:50:ILE:CG2	2.33	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LYS:HB2	1:A:757:PRO:CD	2.18	0.73
1:B:309:ASP:H	1:B:672:ASN:HD21	1.37	0.73
1:B:108:HIS:CE1	1:B:189:GLU:OE1	2.21	0.72
1:A:622:ASN:N	1:A:622:ASN:HD22	1.85	0.72
1:A:449:VAL:HG23	1:A:450:LEU:HD13	1.72	0.71
1:B:783:ASN:HD22	1:B:785:VAL:H	1.36	0.71
1:A:102:ASN:HD22	1:A:102:ASN:H	1.39	0.70
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.40	0.70
1:B:994:ASN:HB3	1:B:997:GLU:HB2	1.74	0.70
1:B:860:GLU:OE2	1:B:957:HIS:HE1	1.76	0.69
1:A:711:ARG:HH21	1:A:711:ARG:HG2	1.59	0.68
1:B:243:LYS:NZ	1:B:243:LYS:HB2	2.09	0.67
1:B:257:VAL:HG21	1:B:437:ILE:HG22	1.76	0.67
1:A:623:THR:OG1	1:A:626:GLY:O	2.06	0.67
1:B:196:ASN:ND2	1:B:198:ALA:H	1.93	0.67
1:B:112:HIS:CE1	1:B:189:GLU:OE1	2.39	0.67
1:B:776:TRP:CD1	1:B:953:LYS:HG2	2.30	0.67
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.43	0.66
1:B:587:PRO:HD3	1:B:695:TRP:CE2	2.30	0.66
1:A:783:ASN:ND2	1:A:786:HIS:H	1.95	0.65
1:A:191:GLU:HA	1:A:194:VAL:HG23	1.79	0.65
1:B:86:SER:HB3	1:B:158:LEU:HG	1.79	0.65
1:A:760:PRO:HA	1:A:763:LEU:HD12	1.77	0.65
1:B:622:ASN:HD22	1:B:622:ASN:N	1.91	0.65
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.32	0.64
1:B:920:ARG:O	1:B:924:GLU:HG3	1.98	0.63
1:A:67:LEU:CD2	1:A:75:VAL:HB	2.29	0.63
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.82	0.62
1:B:575:ASN:N	1:B:575:ASN:HD22	1.96	0.62
1:B:294:GLN:H	1:B:297:HIS:HD2	1.45	0.62
1:B:311:ARG:NH1	1:B:379:LEU:O	2.30	0.62
1:B:309:ASP:H	1:B:672:ASN:ND2	1.96	0.62
1:B:676:GLU:HA	1:B:676:GLU:OE1	1.99	0.62
1:A:294:GLN:H	1:A:297:HIS:CD2	2.16	0.62
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.82	0.61
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.82	0.61
1:B:102:ASN:H	1:B:102:ASN:HD22	1.48	0.61
1:A:545:THR:HB	1:A:546:PRO:HD2	1.82	0.61
1:A:108:HIS:CE1	1:A:189:GLU:OE2	2.50	0.60
1:A:715:PHE:CZ	1:A:719:LEU:HD22	2.36	0.60
1:B:110:LEU:HD23	1:B:110:LEU:C	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:LEU:CD2	1:A:995:MET:HG2	2.32	0.60
1:B:272:VAL:O	1:B:276:SER:OG	2.20	0.60
1:A:616:LEU:HD21	1:A:638:GLN:HG3	1.83	0.60
1:A:491:ARG:CG	1:A:491:ARG:HH11	2.10	0.59
1:A:62:ARG:HG2	1:A:80:ASP:HB2	1.84	0.59
1:A:800:GLN:HB3	1:A:805:ASN:HD21	1.68	0.59
1:B:93:HIS:HD2	1:B:145:GLU:O	1.86	0.59
1:A:303:LYS:HG2	1:A:485:PHE:CE2	2.38	0.58
1:B:693:VAL:HB	1:B:766:TYR:CE2	2.39	0.58
1:A:784:GLU:O	1:A:961:ARG:HG3	2.03	0.58
1:B:962:GLU:OE2	1:B:962:GLU:HA	2.03	0.58
1:A:298:LEU:HD13	1:A:475:ASN:CB	2.33	0.58
1:B:176:GLU:OE1	1:B:179:LYS:NZ	2.37	0.58
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.37	0.58
1:A:309:ASP:H	1:A:672:ASN:ND2	2.01	0.58
1:A:136:GLY:CA	1:A:152:ASP:O	2.52	0.57
1:A:316:THR:HB	1:A:374:ILE:HG22	1.86	0.57
1:B:783:ASN:ND2	1:B:785:VAL:H	2.02	0.57
1:A:185:ALA:HB2	1:A:828:GLN:HE22	1.70	0.57
1:A:341:GLU:OE1	2:A:1101:MGK:H10	2.05	0.57
1:A:688:LEU:HD13	1:A:696:THR:HG22	1.87	0.57
1:B:803:SER:HB2	1:B:927:TYR:OH	2.04	0.57
1:B:298:LEU:HD13	1:B:475:ASN:HB2	1.86	0.57
1:A:674:ARG:HD3	4:A:1235:HOH:O	2.05	0.57
1:A:715:PHE:CZ	1:A:719:LEU:CD2	2.88	0.57
1:B:134:HIS:CD2	1:B:157:HIS:CD2	2.93	0.57
1:B:386:HIS:HD2	1:B:389:ASP:OD2	1.87	0.56
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.40	0.56
1:A:817:GLU:HG3	1:A:818:PRO:CD	2.32	0.56
1:B:765:ARG:NH1	1:B:912:ILE:O	2.39	0.56
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.88	0.56
1:B:535:PHE:HB3	1:B:570:PRO:HG3	1.87	0.56
1:A:722:ARG:HA	1:A:756:LYS:O	2.05	0.55
1:B:887:GLN:HE21	1:B:891:ILE:HD11	1.72	0.55
1:B:941:LYS:HB2	1:B:941:LYS:NZ	2.20	0.55
1:A:780:GLN:HE22	1:A:959:LEU:HD11	1.72	0.55
1:A:363:GLN:HG3	1:A:371:MET:HE1	1.87	0.55
1:A:599:LEU:HD23	1:A:662:ILE:HD13	1.89	0.55
1:A:689:LEU:HD23	1:A:995:MET:HG2	1.87	0.55
1:B:579:PHE:HE2	1:B:765:ARG:HH22	1.55	0.55
1:A:136:GLY:HA2	1:A:152:ASP:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LEU:CD1	1:B:138:SER:HB2	2.36	0.55
1:A:887:GLN:HE21	1:A:891:ILE:HD11	1.72	0.55
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.23	0.54
1:A:425:LYS:NZ	1:A:425:LYS:HB3	2.22	0.54
1:A:874:ILE:HG22	1:A:937:ILE:HD11	1.90	0.54
1:B:538:LEU:HD22	1:B:734:THR:HG23	1.90	0.54
1:B:685:TYR:CZ	1:B:781:GLN:HG3	2.43	0.54
1:B:852:SER:HB3	1:B:859:LEU:HD21	1.90	0.54
1:B:856:PRO:HA	1:B:859:LEU:HB2	1.90	0.54
1:A:329:ASN:N	1:A:330:PRO:CD	2.71	0.54
1:B:108:HIS:O	1:B:111:GLN:HB3	2.08	0.54
1:A:298:LEU:HD13	1:A:475:ASN:HB2	1.90	0.53
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.88	0.53
1:A:602:ASP:OD2	1:A:658:ARG:NH1	2.42	0.53
1:B:262:GLU:CD	1:B:262:GLU:H	2.12	0.53
1:A:880:GLU:HB3	1:B:457:GLU:HG2	1.90	0.53
1:B:685:TYR:HB2	1:B:956:VAL:HG11	1.90	0.53
1:A:482:SER:HB3	1:A:485:PHE:CE1	2.43	0.53
1:B:643:LYS:O	1:B:647:GLU:HB2	2.09	0.53
1:B:783:ASN:ND2	1:B:786:HIS:H	2.07	0.53
1:B:203:GLN:HG3	1:B:203:GLN:O	2.08	0.53
1:B:815:ILE:HG22	1:B:870:MET:HG2	1.91	0.53
1:B:809:GLU:OE2	1:B:839:ARG:NH2	2.39	0.53
1:B:459:PHE:CE2	1:B:461:PRO:HG3	2.43	0.53
2:B:1101:MGK:O14	2:B:1101:MGK:C26	2.55	0.53
1:B:807:PHE:HE1	1:B:935:ASP:HB3	1.73	0.53
1:A:97:LEU:HB2	1:A:144:GLY:O	2.09	0.53
1:B:772:PRO:HD3	1:B:1002:LEU:HD21	1.91	0.53
1:A:78:ILE:O	1:A:259:LEU:HA	2.09	0.52
1:B:583:ALA:CB	1:B:626:GLY:HA2	2.39	0.52
1:B:887:GLN:O	1:B:890:ALA:HB3	2.09	0.52
1:A:428:GLU:H	1:A:428:GLU:CD	2.12	0.52
1:A:599:LEU:HD21	1:A:659:PHE:HA	1.91	0.52
1:A:756:LYS:HB2	1:A:757:PRO:HD2	1.92	0.52
1:B:134:HIS:HD2	1:B:157:HIS:CD2	2.28	0.52
1:B:774:ARG:HG3	1:B:774:ARG:NH1	2.04	0.52
2:A:1101:MGK:H08	2:A:1101:MGK:HN12	1.74	0.52
1:A:188:SER:HB3	1:A:831:TYR:CB	2.35	0.52
1:A:805:ASN:O	1:A:809:GLU:HG3	2.09	0.52
1:B:774:ARG:CG	1:B:774:ARG:NH1	2.66	0.52
1:B:196:ASN:ND2	1:B:198:ALA:N	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.92	0.52
1:B:575:ASN:ND2	1:B:575:ASN:N	2.57	0.52
1:A:67:LEU:HD23	1:A:75:VAL:HB	1.92	0.51
1:B:108:HIS:HE1	1:B:189:GLU:CD	2.08	0.51
1:B:444:TYR:CE1	1:B:452:ALA:HB1	2.46	0.51
1:A:350:LEU:HB3	1:A:356:VAL:HG22	1.91	0.51
1:A:620:LEU:HD13	1:A:629:LEU:HG	1.92	0.51
1:A:714:ALA:O	1:A:717:PRO:HD2	2.11	0.51
1:B:194:VAL:HG12	1:B:195:MET:HG2	1.91	0.51
1:B:184:ASN:HD21	1:B:223:LYS:NZ	2.09	0.51
1:A:511:LYS:HE3	1:A:514:GLN:OE1	2.11	0.51
1:A:595:LEU:HD12	1:A:662:ILE:HG22	1.92	0.51
1:B:298:LEU:HD21	1:B:318:PRO:HG3	1.93	0.51
1:B:843:ILE:HG22	1:B:844:GLN:N	2.25	0.51
1:A:334:LEU:HD22	1:A:468:LEU:HD13	1.93	0.50
1:B:817:GLU:N	1:B:818:PRO:HD2	2.25	0.50
1:A:693:VAL:HB	1:A:766:TYR:CE2	2.45	0.50
1:B:583:ALA:HB2	1:B:626:GLY:HA2	1.93	0.50
1:B:600:LEU:HD11	1:B:648:LYS:HB3	1.93	0.50
1:B:803:SER:HB2	1:B:927:TYR:CZ	2.46	0.50
1:A:108:HIS:CE1	1:A:189:GLU:CD	2.84	0.50
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.47	0.50
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.15	0.50
1:B:889:LEU:HB3	1:B:928:LEU:HD11	1.94	0.50
1:A:196:ASN:ND2	1:A:196:ASN:C	2.64	0.50
1:B:229:ARG:NH1	1:B:233:GLU:OE2	2.41	0.50
1:A:196:ASN:HD22	1:A:199:TRP:H	1.60	0.50
1:B:175:ASP:HB3	1:B:178:ALA:HB3	1.93	0.50
1:B:196:ASN:HD22	1:B:196:ASN:C	2.15	0.50
1:B:52:ASN:HD22	1:B:52:ASN:N	2.09	0.50
1:B:587:PRO:HD3	1:B:695:TRP:CD2	2.46	0.50
1:B:708:THR:OG1	1:B:711:ARG:HB2	2.11	0.50
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.94	0.49
1:A:86:SER:HB3	1:A:158:LEU:HG	1.94	0.49
1:B:815:ILE:HA	1:B:870:MET:HE2	1.93	0.49
1:B:118:THR:HG21	1:B:167:GLN:HB3	1.93	0.49
1:B:346:LEU:HA	1:B:522:PHE:HE2	1.76	0.49
1:B:795:TYR:CE2	1:B:953:LYS:HD2	2.48	0.49
1:B:413:GLU:OE2	1:B:527:LYS:HE2	2.12	0.49
1:B:214:PRO:O	1:B:217:LYS:HG3	2.13	0.49
1:A:586:ASP:HA	1:A:695:TRP:CZ2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:HG2	1:B:80:ASP:HB2	1.94	0.49
1:B:940:TYR:CE1	1:B:945:ALA:HB2	2.48	0.49
1:A:886:ILE:HG23	1:A:928:LEU:HD13	1.95	0.49
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.95	0.48
1:A:312:ASN:HB3	1:A:377:VAL:O	2.13	0.48
1:B:359:LEU:O	2:B:1101:MGK:H10	2.13	0.48
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.95	0.48
1:B:643:LYS:HB2	1:B:744:MET:SD	2.53	0.48
1:B:304:ILE:HB	1:B:481:VAL:HG22	1.95	0.48
1:B:196:ASN:HD22	1:B:198:ALA:N	2.11	0.48
1:B:874:ILE:HA	1:B:877:MET:HG2	1.94	0.48
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.44	0.48
1:A:793:ILE:O	1:A:847:ARG:HA	2.14	0.48
1:B:189:GLU:HG2	1:B:831:TYR:CD1	2.47	0.48
1:B:125:ASN:H	1:B:125:ASN:HD22	1.62	0.48
1:B:655:ASP:HB3	1:B:658:ARG:HB2	1.96	0.48
1:B:329:ASN:HD22	1:B:332:HIS:H	1.60	0.47
1:B:559:LEU:HD22	1:B:742:MET:HB2	1.95	0.47
1:A:521:LYS:HD2	1:A:521:LYS:HA	1.58	0.47
1:A:908:TRP:O	1:A:912:ILE:HG12	2.15	0.47
2:B:1101:MGK:H18A	2:B:1101:MGK:H15A	1.75	0.47
1:B:622:ASN:H	1:B:622:ASN:ND2	2.03	0.47
1:B:686:LEU:HA	1:B:686:LEU:HD12	1.66	0.47
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.62	0.47
1:B:243:LYS:HZ2	1:B:243:LYS:HB2	1.80	0.47
1:B:579:PHE:HE2	1:B:765:ARG:NH2	2.11	0.47
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.97	0.47
1:A:298:LEU:HD13	1:A:475:ASN:HB3	1.95	0.47
1:B:52:ASN:ND2	1:B:52:ASN:N	2.62	0.47
1:B:600:LEU:O	1:B:604:LEU:HB2	2.14	0.47
1:A:363:GLN:HG3	1:A:371:MET:CE	2.44	0.47
1:B:616:LEU:HD21	1:B:638:GLN:HG3	1.97	0.47
1:A:196:ASN:ND2	1:A:199:TRP:H	2.13	0.47
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.48	0.47
1:A:359:LEU:HD23	1:A:359:LEU:C	2.36	0.47
1:A:852:SER:HB3	1:A:859:LEU:HD21	1.96	0.47
1:A:756:LYS:CB	1:A:757:PRO:CD	2.88	0.46
1:A:780:GLN:O	1:A:781:GLN:HG2	2.16	0.46
1:B:602:ASP:OD1	1:B:658:ARG:HD3	2.16	0.46
1:A:583:ALA:CB	1:A:626:GLY:HA2	2.44	0.46
1:B:250:SER:HB2	1:B:281:LYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:SER:HB3	1:B:831:TYR:HB2	1.97	0.46
1:A:782:ARG:NH1	1:A:963:MET:O	2.45	0.46
1:B:597:LEU:HD21	1:B:627:MET:HG2	1.97	0.46
1:B:90:LEU:HD12	1:B:256:VAL:HG22	1.98	0.46
1:A:392:LEU:O	1:A:396:GLN:HG3	2.15	0.46
1:A:880:GLU:CG	1:B:457:GLU:HG2	2.45	0.46
1:B:671:ASN:OD1	1:B:701:LYS:HD3	2.16	0.46
1:B:932:THR:OG1	1:B:934:GLU:HB2	2.16	0.46
1:A:102:ASN:HD22	1:A:102:ASN:N	2.06	0.46
1:A:140:ALA:HA	1:A:148:ASN:O	2.16	0.46
1:A:914:GLN:HA	1:A:916:TYR:CE1	2.51	0.46
1:A:789:SER:HB2	1:A:958:VAL:O	2.16	0.46
1:B:809:GLU:OE1	1:B:893:ARG:HD3	2.16	0.46
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.98	0.45
1:A:313:LEU:HD22	1:A:387:VAL:HG22	1.98	0.45
1:A:906:LYS:NZ	1:A:921:ASP:OD2	2.49	0.45
1:B:200:ARG:NH2	1:B:498:THR:HA	2.32	0.45
1:B:861:SER:O	1:B:865:ALA:N	2.48	0.45
1:B:622:ASN:ND2	1:B:622:ASN:N	2.63	0.45
1:B:691:THR:O	1:B:999:LYS:CE	2.65	0.45
1:B:915:GLN:HG2	1:B:1008:VAL:HG11	1.99	0.45
1:A:597:LEU:HD12	1:A:597:LEU:HA	1.63	0.45
1:B:672:ASN:HA	1:B:672:ASN:HD22	1.53	0.45
1:B:838:ARG:HG3	1:B:847:ARG:HD3	1.98	0.45
1:A:773:ASP:O	1:A:774:ARG:HB2	2.17	0.45
1:B:308:LYS:HD3	1:B:672:ASN:HB3	1.98	0.45
1:A:600:LEU:HD11	1:A:648:LYS:HB3	1.97	0.45
1:A:706:ASP:O	1:A:711:ARG:HD3	2.15	0.44
1:B:948:ALA:HB3	1:B:951:ARG:HB2	1.99	0.44
1:A:756:LYS:CB	1:A:757:PRO:HD3	2.47	0.44
1:B:229:ARG:HD3	1:B:229:ARG:HA	1.54	0.44
1:B:578:PHE:CD2	1:B:725:ILE:HG12	2.52	0.44
1:B:76:LEU:HD12	1:B:437:ILE:HG21	1.99	0.44
1:A:756:LYS:HB2	1:A:757:PRO:HD3	1.97	0.44
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.20	0.44
1:B:341:GLU:HG2	1:B:347:LEU:CD1	2.25	0.44
1:B:770:GLN:HG2	1:B:1003:PRO:HG2	1.98	0.44
1:B:810:LEU:HG	1:B:928:LEU:HD21	2.00	0.44
1:B:941:LYS:HZ1	1:B:941:LYS:HB2	1.82	0.44
1:B:583:ALA:O	1:B:590:SER:HA	2.17	0.44
1:A:206:LYS:HB3	1:A:216:SER:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:LEU:HD21	1:A:995:MET:HG2	1.99	0.44
1:B:196:ASN:ND2	1:B:196:ASN:C	2.71	0.44
1:B:826:LYS:HE3	1:B:826:LYS:HB2	1.61	0.44
1:B:349:GLU:HA	1:B:349:GLU:OE2	2.18	0.44
1:B:946:VAL:HA	1:B:951:ARG:CZ	2.48	0.44
1:A:123:LYS:O	1:A:124:GLU:C	2.56	0.44
1:A:824:ARG:O	1:A:828:GLN:HA	2.18	0.44
1:B:294:GLN:H	1:B:297:HIS:CD2	2.31	0.44
1:A:294:GLN:O	1:A:298:LEU:HG	2.18	0.43
1:A:334:LEU:CD2	1:A:468:LEU:HD13	2.48	0.43
1:B:425:LYS:HB3	1:B:425:LYS:HE3	1.82	0.43
1:B:744:MET:O	1:B:744:MET:HG2	2.17	0.43
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.80	0.43
1:A:583:ALA:HB2	1:A:626:GLY:HA2	1.99	0.43
1:B:329:ASN:ND2	1:B:332:HIS:CB	2.81	0.43
1:A:1009:LYS:HD2	1:A:1009:LYS:HA	1.80	0.43
1:A:886:ILE:HG12	1:A:928:LEU:HD22	2.00	0.43
1:B:329:ASN:ND2	1:B:332:HIS:HB2	2.33	0.43
1:B:363:GLN:HG3	1:B:371:MET:CE	2.49	0.43
1:B:656:GLU:O	1:B:659:PHE:HB3	2.18	0.43
1:A:136:GLY:HA3	1:A:152:ASP:O	2.19	0.43
1:A:67:LEU:C	1:A:67:LEU:HD23	2.38	0.43
1:A:51:GLY:HA2	1:A:52:ASN:HA	1.71	0.43
1:A:862:ARG:NH2	1:A:981:SER:O	2.44	0.43
1:B:785:VAL:HG12	1:B:786:HIS:CD2	2.53	0.43
1:A:125:ASN:HD22	1:A:125:ASN:H	1.66	0.43
1:B:93:HIS:CD2	1:B:145:GLU:O	2.70	0.43
1:A:299:LYS:HB2	1:A:299:LYS:HE3	1.88	0.43
1:A:887:GLN:HE21	1:A:891:ILE:CD1	2.32	0.43
1:A:806:MET:CE	1:A:928:LEU:HG	2.49	0.43
1:B:160:GLY:O	1:B:164:ARG:HG3	2.18	0.43
1:B:78:ILE:O	1:B:259:LEU:HA	2.19	0.43
1:B:962:GLU:OE2	1:B:962:GLU:CA	2.66	0.43
1:B:170:LEU:HA	1:B:170:LEU:HD23	1.61	0.43
1:B:311:ARG:HB3	1:B:379:LEU:HB2	2.01	0.43
1:A:809:GLU:HB3	1:A:889:LEU:HD11	2.01	0.43
1:A:567:PHE:CE1	1:A:900:LEU:HA	2.53	0.43
1:B:597:LEU:HD23	1:B:622:ASN:N	2.34	0.43
1:A:336:HIS:HD2	1:A:337:LEU:HD13	1.84	0.42
1:A:441:LEU:HA	1:A:441:LEU:HD23	1.85	0.42
1:B:129:GLN:O	1:B:133:GLU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.52	0.42
1:B:631:VAL:HG12	1:B:638:GLN:HG2	2.01	0.42
1:B:674:ARG:CG	1:B:674:ARG:HH11	2.32	0.42
1:A:441:LEU:CD2	1:A:449:VAL:HG11	2.48	0.42
1:A:460:ARG:HD2	1:A:462:ASP:OD2	2.18	0.42
1:A:596:TYR:OH	1:A:649:MET:HG3	2.19	0.42
1:A:896:LYS:HE2	1:A:896:LYS:HB2	1.52	0.42
1:B:511:LYS:HD2	1:B:514:GLN:OE1	2.19	0.42
1:A:408:GLU:HB2	1:A:459:PHE:CE2	2.55	0.42
1:B:730:HIS:HD2	1:B:904:SER:OG	2.02	0.42
1:A:114:LEU:HD13	1:A:168:PHE:HB3	2.01	0.42
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.75	0.42
1:A:799:MET:HG2	1:A:843:ILE:CD1	2.50	0.42
1:A:187:ASP:O	1:A:191:GLU:HG2	2.20	0.42
1:A:586:ASP:OD1	1:A:589:HIS:HD2	2.01	0.42
1:A:774:ARG:NH1	1:A:774:ARG:HG3	2.34	0.42
1:A:780:GLN:NE2	1:A:959:LEU:HD11	2.34	0.42
1:B:243:LYS:HE2	4:B:1206:HOH:O	2.20	0.42
1:A:584:TYR:CE2	1:A:624:ILE:HG22	2.55	0.41
1:B:817:GLU:N	1:B:818:PRO:CD	2.83	0.41
1:A:709:LEU:O	1:A:710:PRO:C	2.59	0.41
1:A:691:THR:HG23	1:A:841:ASN:HD21	1.85	0.41
1:B:767:ARG:HG2	1:B:1007:LEU:HD13	2.02	0.41
1:B:445:PRO:HG2	1:B:448:GLU:HG3	2.01	0.41
1:A:559:LEU:HD22	1:A:742:MET:HB2	2.02	0.41
1:B:238:ARG:O	1:B:242:LEU:HD12	2.20	0.41
1:A:359:LEU:HD23	1:A:360:VAL:N	2.36	0.41
1:B:114:LEU:HD12	1:B:149:TYR:CZ	2.56	0.41
1:B:417:LEU:HA	1:B:417:LEU:HD12	1.69	0.41
1:A:547:TYR:HB2	4:A:1202:HOH:O	2.20	0.41
1:B:433:TYR:CE1	1:B:437:ILE:HD11	2.55	0.41
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.55	0.41
1:A:584:TYR:CZ	1:A:624:ILE:HG22	2.55	0.41
1:A:941:LYS:O	1:A:949:PRO:HD2	2.21	0.41
1:A:652:PHE:CE2	1:A:654:ILE:HG12	2.55	0.41
1:A:94:ILE:HG22	1:A:95:GLY:N	2.35	0.41
1:A:1004:LEU:HA	1:A:1004:LEU:HD23	1.88	0.41
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.63	0.41
1:B:329:ASN:O	1:B:330:PRO:C	2.56	0.41
1:B:465:GLU:O	1:B:469:ASP:HB2	2.20	0.41
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:NZ	4:A:1255:HOH:O	2.53	0.41
1:A:852:SER:OG	1:A:853:GLU:N	2.54	0.41
1:B:202:PHE:CZ	1:B:206:LYS:HE3	2.55	0.41
1:A:196:ASN:C	1:A:196:ASN:HD22	2.24	0.41
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.54	0.41
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.21	0.40
1:A:151:PHE:C	1:A:151:PHE:CD1	2.94	0.40
1:A:204:LEU:O	1:A:208:THR:HG23	2.22	0.40
1:B:773:ASP:O	1:B:774:ARG:HB2	2.21	0.40
1:A:164:ARG:HH11	1:A:164:ARG:HG3	1.85	0.40
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.57	0.40
1:B:801:SER:O	1:B:802:THR:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	951/990 (96%)	893 (94%)	55 (6%)	3 (0%)	44	81
1	B	951/990 (96%)	891 (94%)	57 (6%)	3 (0%)	44	81
All	All	1902/1980 (96%)	1784 (94%)	112 (6%)	6 (0%)	44	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	ASP
1	A	961	ARG
1	A	841	ASN
1	B	841	ASN
1	B	1010	PRO
1	B	520	GLY

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	848/879 (96%)	741 (87%)	107 (13%)	5	23
1	B	846/879 (96%)	730 (86%)	116 (14%)	4	19
All	All	1694/1758 (96%)	1471 (87%)	223 (13%)	5	20

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	52	ASN
1	A	61	LYS
1	A	67	LEU
1	A	76	LEU
1	A	97	LEU
1	A	102	ASN
1	A	111	GLN
1	A	120	LYS
1	A	125	ASN
1	A	148	ASN
1	A	156	GLU
1	A	158	LEU
1	A	188	SER
1	A	196	ASN
1	A	201	LEU
1	A	226	LEU
1	A	239	GLN
1	A	270	LEU
1	A	277	GLU
1	A	285	LEU
1	A	287	GLU
1	A	303	LYS
1	A	312	ASN
1	A	316	THR
1	A	324	LYS
1	A	329	ASN

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Mol	Chain	Res	Type
1	A	332	HIS
1	A	337	LEU
1	A	347	LEU
1	A	353	LYS
1	A	360	VAL
1	A	363	GLN
1	A	364	LYS
1	A	402	ARG
1	A	412	GLN
1	A	414	LEU
1	A	417	LEU
1	A	420	VAL
1	A	423	ARG
1	A	433	TYR
1	A	446	LEU
1	A	466	MET
1	A	488	LYS
1	A	489	THR
1	A	491	ARG
1	A	501	LYS
1	A	508	GLU
1	A	511	LYS
1	A	517	ASP
1	A	521	LYS
1	A	524	LEU
1	A	527	LYS
1	A	538	LEU
1	A	558	LYS
1	A	595	LEU
1	A	597	LEU
1	A	607	TYR
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	642	LEU
1	A	644	LYS
1	A	648	LYS
1	A	657	LYS
1	A	662	ILE
1	A	663	LYS
1	A	674	ARG
1	A	677	GLN

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Mol	Chain	Res	Type
1	A	691	THR
1	A	711	ARG
1	A	712	LEU
1	A	719	LEU
1	A	722	ARG
1	A	728	LEU
1	A	741	ILE
1	A	744	MET
1	A	751	GLU
1	A	756	LYS
1	A	758	LEU
1	A	759	LEU
1	A	764	VAL
1	A	765	ARG
1	A	771	LEU
1	A	780	GLN
1	A	783	ASN
1	A	801	SER
1	A	810	LEU
1	A	823	LEU
1	A	838	ARG
1	A	846	LEU
1	A	859	LEU
1	A	862	ARG
1	A	867	LEU
1	A	872	LYS
1	A	889	LEU
1	A	892	ARG
1	A	901	SER
1	A	906	LYS
1	A	928	LEU
1	A	929	LYS
1	A	933	LYS
1	A	938	LYS
1	A	957	HIS
1	A	982	GLN
1	A	1007	LEU
1	A	1011	HIS
1	B	44	ASN
1	B	61	LYS
1	B	76	LEU
1	B	92	VAL

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Mol	Chain	Res	Type
1	B	97	LEU
1	B	102	ASN
1	B	111	GLN
1	B	119	LYS
1	B	125	ASN
1	B	128	SER
1	B	148	ASN
1	B	158	LEU
1	B	179	LYS
1	B	188	SER
1	B	196	ASN
1	B	201	LEU
1	B	226	LEU
1	B	229	ARG
1	B	239	GLN
1	B	270	LEU
1	B	276	SER
1	B	285	LEU
1	B	287	GLU
1	B	290	GLU
1	B	316	THR
1	B	329	ASN
1	B	337	LEU
1	B	347	LEU
1	B	348	SER
1	B	353	LYS
1	B	360	VAL
1	B	364	LYS
1	B	399	GLN
1	B	414	LEU
1	B	417	LEU
1	B	440	ILE
1	B	446	LEU
1	B	450	LEU
1	B	458	GLU
1	B	460	ARG
1	B	494	GLU
1	B	507	ASP
1	B	508	GLU
1	B	512	LYS
1	B	517	ASP
1	B	521	LYS

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Mol	Chain	Res	Type
1	B	523	LYS
1	B	524	LEU
1	B	527	LYS
1	B	556	MET
1	B	575	ASN
1	B	586	ASP
1	B	587	PRO
1	B	595	LEU
1	B	597	LEU
1	B	601	LYS
1	B	602	ASP
1	B	604	LEU
1	B	612	GLU
1	B	616	LEU
1	B	622	ASN
1	B	629	LEU
1	B	642	LEU
1	B	643	LYS
1	B	644	LYS
1	B	648	LYS
1	B	657	LYS
1	B	674	ARG
1	B	677	GLN
1	B	702	GLU
1	B	711	ARG
1	B	712	LEU
1	B	713	LYS
1	B	718	GLN
1	B	728	LEU
1	B	733	ILE
1	B	736	GLN
1	B	744	MET
1	B	746	GLU
1	B	751	GLU
1	B	756	LYS
1	B	759	LEU
1	B	764	VAL
1	B	765	ARG
1	B	774	ARG
1	B	782	ARG
1	B	783	ASN
1	B	803	SER

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Mol	Chain	Res	Type
1	B	806	MET
1	B	809	GLU
1	B	810	LEU
1	B	823	LEU
1	B	838	ARG
1	B	846	LEU
1	B	854	LYS
1	B	859	LEU
1	B	867	LEU
1	B	868	ILE
1	B	880	GLU
1	B	884	LYS
1	B	886	ILE
1	B	889	LEU
1	B	892	ARG
1	B	898	LYS
1	B	899	LYS
1	B	923	THR
1	B	928	LEU
1	B	941	LYS
1	B	942	GLU
1	B	957	HIS
1	B	980	LEU
1	B	990	GLU
1	B	993	GLN
1	B	1007	LEU
1	B	1009	LYS
1	B	1011	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	53	HIS
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	148	ASN
1	A	196	ASN
1	A	231	ASN
1	A	232	GLN
1	A	297	HIS

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Mol	Chain	Res	Type
1	A	300	GLN
1	A	329	ASN
1	A	336	HIS
1	A	393	HIS
1	A	407	GLN
1	A	502	GLN
1	A	575	ASN
1	A	589	HIS
1	A	605	ASN
1	A	622	ASN
1	A	672	ASN
1	A	730	HIS
1	A	770	GLN
1	A	780	GLN
1	A	783	ASN
1	A	786	HIS
1	A	805	ASN
1	A	828	GLN
1	A	841	ASN
1	A	887	GLN
1	A	988	GLN
1	B	52	ASN
1	B	93	HIS
1	B	102	ASN
1	B	111	GLN
1	B	125	ASN
1	B	134	HIS
1	B	148	ASN
1	B	157	HIS
1	B	184	ASN
1	B	196	ASN
1	B	231	ASN
1	B	232	GLN
1	B	297	HIS
1	B	300	GLN
1	B	329	ASN
1	B	336	HIS
1	B	386	HIS
1	B	475	ASN
1	B	502	GLN
1	B	575	ASN
1	B	589	HIS

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Mol	Chain	Res	Type
1	B	622	ASN
1	B	672	ASN
1	B	730	HIS
1	B	783	ASN
1	B	805	ASN
1	B	821	ASN
1	B	828	GLN
1	B	841	ASN
1	B	883	GLN
1	B	887	GLN
1	B	922	ASN
1	B	957	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	MGK	A	1101	-	23,30,30	1.62	2 (8%)	29,38,38	2.06	6 (20%)
2	MGK	B	1101	-	23,30,30	1.73	3 (13%)	29,38,38	1.96	7 (24%)

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	MGK	A	1101	-	-	0/26/28/28	0/2/2/2
2	MGK	B	1101	-	-	0/26/28/28	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	MGK	C21-C20	2.06	1.43	1.38
2	A	1101	MGK	C26-N16	2.17	1.51	1.47
2	B	1101	MGK	C26-N16	2.69	1.52	1.47
2	A	1101	MGK	O02-C03	6.22	1.49	1.33
2	B	1101	MGK	O02-C03	6.39	1.49	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	MGK	O04-C03-C05	-2.51	116.42	123.91
2	B	1101	MGK	O02-C03-O04	-2.51	118.77	123.82
2	A	1101	MGK	O14-C13-N12	-2.10	119.34	122.97
2	B	1101	MGK	C26-N16-C17	2.26	116.09	111.29
2	B	1101	MGK	C03-C05-N12	2.75	117.15	110.70
2	B	1101	MGK	C05-N12-C13	3.16	129.97	121.62
2	A	1101	MGK	C15-C13-N12	3.69	122.50	115.17
2	A	1101	MGK	C01-O02-C03	4.00	125.35	115.97
2	B	1101	MGK	C01-O02-C03	4.07	125.52	115.97
2	A	1101	MGK	O02-C03-C05	4.30	122.90	111.54
2	B	1101	MGK	O02-C03-C05	4.42	123.21	111.54
2	B	1101	MGK	C27-C26-N16	5.36	121.11	113.48
2	A	1101	MGK	C27-C26-N16	6.72	123.05	113.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	MGK	2	0
2	B	1101	MGK	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	955/990 (96%)	-0.59	0 100 100	19, 34, 50, 77	0
1	B	955/990 (96%)	-0.53	0 100 100	24, 38, 55, 75	0
All	All	1910/1980 (96%)	-0.56	0 100 100	19, 36, 52, 77	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MGK	B	1101	29/29	0.76	0.32	9.01	73,81,100,101	0
2	MGK	A	1101	29/29	0.88	0.24	4.82	61,78,92,92	0
3	ZN	B	1102	1/1	0.87	0.21	-	2,2,2,2	0
3	ZN	A	1102	1/1	0.95	0.23	-	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.