



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 10:29 AM EDT

PDB ID : 7K1D
Title : Crystal structure of human insulin degrading enzyme (IDE) in complex with compound BDM_77291
Authors : Liang, W.G.; Deprez, R.; Bosc, D.; Tang, W.
Deposited on : 2020-09-07
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

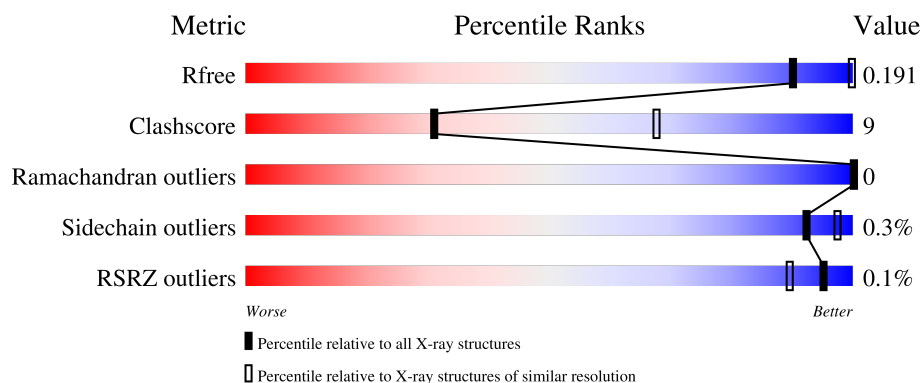
1 Overall quality at a glance

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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	990	 75% 21% •
1	B	990	 79% 17% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15889 atoms, of which 82 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	957	Total	C	N	O	S	0	0	0
			7829	5042	1314	1451	22			
1	B	958	Total	C	N	O	S	0	0	0
			7834	5047	1315	1449	23			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	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	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
A	974	ALA	CYS	engineered mutation	UNP P14735

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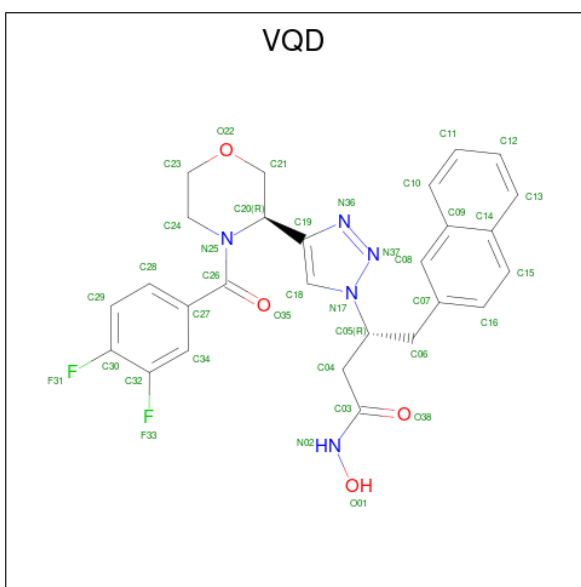
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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	initiating methionine	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	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	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 ZINC ION (three-letter code: ZN) (formula: Zn).

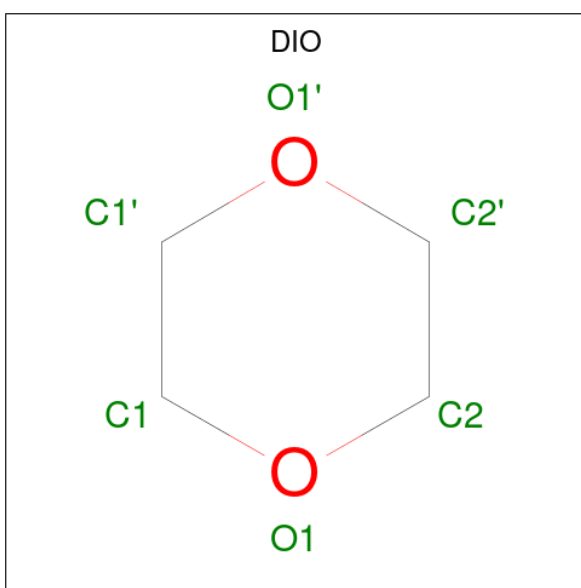
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is (3R)-3-{4-[(3R)-4-(3,4-difluorobenzene-1-carbonyl)morpholin-3-yl]-1H-1,2,3-triazol-1-yl}-N-hydroxy-4-(naphthalen-2-yl)butanamide (three-letter code: VQD) (formula: C₂₇H₂₅F₂N₅O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			38	27	2	5	4		
3	B	1	Total	C	F	N	O	0	0
			38	27	2	5	4		

- Molecule 4 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



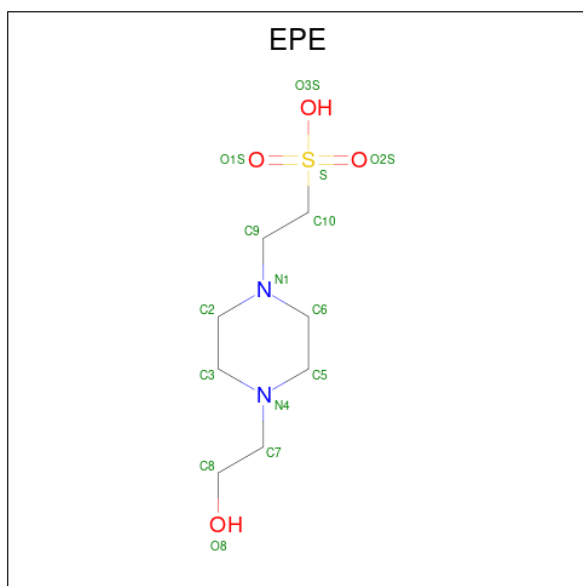
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	4	8	2		
4	A	1	Total	C	H	O	0	0
			14	4	8	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	4	8	2		
4	B	1	Total	C	H	O	0	0
			14	4	8	2		
4	B	1	Total	C	H	O	0	0
			14	4	8	2		
4	B	1	Total	C	H	O	0	0
			14	4	8	2		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).

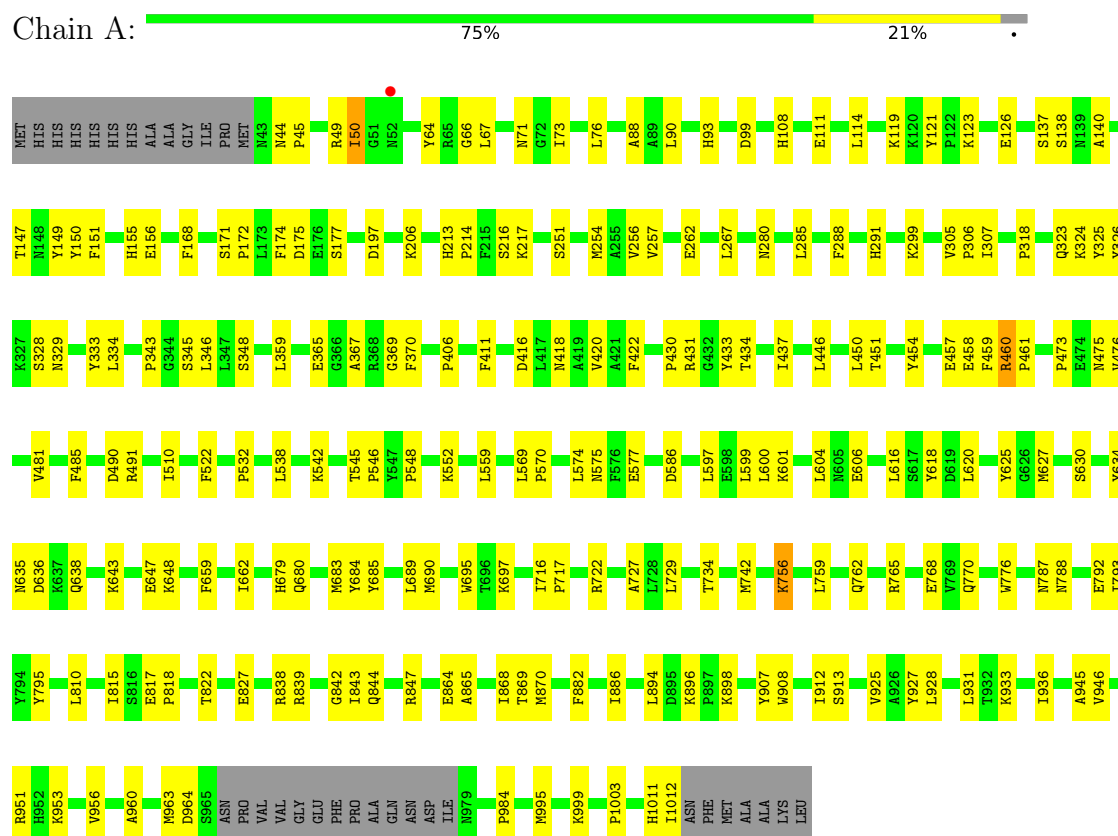


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
5	B	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

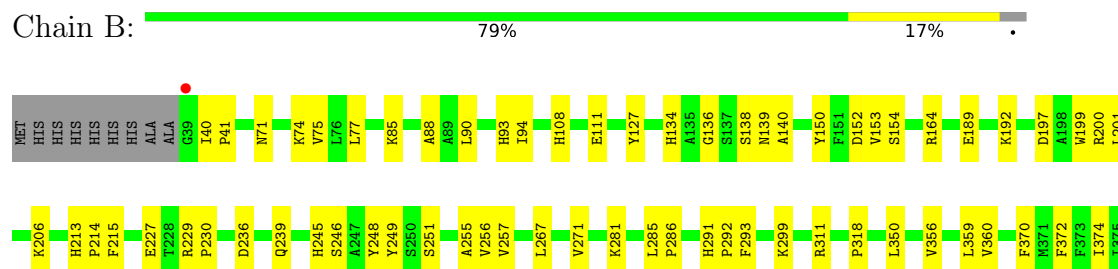
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Insulin-degrading enzyme



• Molecule 1: Insulin-degrading enzyme



N376	E598	W776	E962
L392	L599	F777	N963
Q396	L600	N787	ASP
R431	L604	E792	SER
L441	L616	I793	ASN
V449	L620	Q796	PRO
L450	G626	M799	VAL
T451	L629	L808	VAL
L455	N635	E817	GLY
P473	D636	P818	GLU
V476	K637	F820	PHE
V481	Q638	R824	PRO
S482	K643	I843	ALA
K483	E647	Q844	GLN
E486	K648	G845	ASN
D507	F659	I846	ASP
I510	Q677	R847	N979
K511	M683	I868	L980
T526	T696	K872	P984
K527	E699	W877	E990
L538	L709	L894	V1008
P548	P710	Y907	K1009
K552	A714	Q914	P1010
S557	F715	Q915	H1011
K558	I716	Y916	ILE
L559	P717	V925	ASN
D565	R722	K333	PHE
K566	I725	Y940	MET
L574	L729	K941	ALA
E577	N732	E942	ALA
F578	I733	A945	LYS
F579	T734	V946	LEU
A583	M742	D947	
D586	L758	A948	
P587	L771	P949	
Y594	R774	R950	
	G775	R951	
		H952	
		K953	
		R961	

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	264.31Å 264.31Å 90.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.42 – 3.00 45.42 – 3.00	Depositor EDS
% Data completeness (in resolution range)	75.2 (45.42-3.00) 89.9 (45.42-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.156 , 0.192 0.158 , 0.191	Depositor DCC
R_{free} test set	1990 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15889	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DIO, VQD, EPE, 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	0.47	0/8024	0.63	0/10854
1	B	0.49	0/8030	0.65	0/10862
All	All	0.48	0/16054	0.64	0/21716

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

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	7829	0	7769	162	0
1	B	7834	0	7779	123	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	38	0	0	0	0
3	B	38	0	0	0	0
4	A	18	24	24	0	0
4	B	18	24	24	1	0
5	A	15	17	17	1	0
5	B	15	17	17	0	0
All	All	15807	82	15630	285	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 9.

All (285) 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:153:VAL:HG22	1:B:154:SER:H	1.00	1.15
1:B:153:VAL:HG22	1:B:154:SER:N	1.70	0.98
1:B:153:VAL:CG2	1:B:154:SER:H	1.76	0.98
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.46	0.94
1:A:545:THR:HG22	1:A:546:PRO:HD2	1.50	0.93
1:A:197:ASP:OD1	1:A:306:PRO:HB2	1.68	0.93
1:B:799:MET:HE3	1:B:1008:VAL:HG22	1.51	0.92
1:B:868:ILE:HD12	1:B:984:PRO:HD3	1.53	0.90
1:A:197:ASP:OD1	1:A:306:PRO:CB	2.21	0.88
1:B:134:HIS:O	1:B:153:VAL:HG23	1.76	0.85
1:A:545:THR:CG2	1:A:546:PRO:HD2	2.07	0.84
1:B:557:SER:HB2	1:B:742:MET:CE	2.11	0.81
1:A:93:HIS:CD2	1:A:285:LEU:HD11	2.16	0.81
1:A:119:LYS:HG2	1:A:171:SER:HB2	1.63	0.80
1:A:815:ILE:HG22	1:A:870:MET:HE2	1.64	0.80
1:B:285:LEU:HD12	1:B:286:PRO:HD2	1.66	0.77
1:A:138:SER:HB2	1:A:150:TYR:O	1.84	0.77
1:A:574:LEU:HD22	1:A:729:LEU:HD22	1.66	0.76
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.21	0.76
1:B:134:HIS:O	1:B:153:VAL:CG2	2.33	0.76
1:B:577:GLU:HG2	1:B:579:PHE:CZ	2.23	0.73
1:B:93:HIS:CD2	1:B:285:LEU:HD11	2.25	0.71
1:B:557:SER:HB2	1:B:742:MET:HE2	1.70	0.71
1:A:88:ALA:HB3	1:A:151:PHE:CE2	2.26	0.71
1:A:532:PRO:HG3	1:A:634:TYR:CD2	2.26	0.70
1:A:776:TRP:CD1	1:A:953:LYS:HG2	2.27	0.69
1:A:306:PRO:HG3	1:A:481:VAL:CG1	2.22	0.69
1:A:119:LYS:CG	1:A:171:SER:HB2	2.22	0.69
1:A:490:ASP:OD1	1:A:491:ARG:HG3	1.94	0.66
1:A:111:GLU:OE2	1:A:140:ALA:HB3	1.95	0.66
1:A:604:LEU:HG	1:A:648:LYS:HD2	1.78	0.66
1:A:616:LEU:HD11	1:A:638:GLN:HG2	1.78	0.66
1:A:306:PRO:HD3	1:A:481:VAL:HG13	1.77	0.66
1:B:507:ASP:O	1:B:511:LYS:HG2	1.94	0.66
1:B:111:GLU:OE2	1:B:140:ALA:HB3	1.96	0.65
1:A:324:LYS:HE3	1:A:325:TYR:CZ	2.31	0.65
1:A:868:ILE:HD12	1:A:984:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:817:GLU:HB3	1:B:818:PRO:HD3	1.78	0.65
1:A:963:MET:HG2	1:A:964:ASP:H	1.63	0.64
1:B:799:MET:CE	1:B:1008:VAL:HG22	2.27	0.64
1:B:868:ILE:CD1	1:B:984:PRO:HD3	2.27	0.63
1:A:306:PRO:HG3	1:A:481:VAL:HG12	1.80	0.63
1:B:696:THR:OG1	1:B:699:GLU:HG3	1.98	0.63
1:A:416:ASP:O	1:A:420:VAL:HG23	1.99	0.62
1:B:940:TYR:CE2	1:B:945:ALA:HB2	2.34	0.62
1:B:716:ILE:CB	1:B:717:PRO:HD3	2.24	0.62
1:B:877:MET:O	1:B:933:LYS:NZ	2.31	0.62
1:B:643:LYS:HE2	1:B:647:GLU:OE1	1.99	0.62
1:B:267:LEU:O	1:B:271:VAL:HG23	1.99	0.62
1:A:795:TYR:HE1	1:A:951:ARG:NH2	1.99	0.61
1:B:136:GLY:HA2	1:B:152:ASP:O	2.00	0.61
1:A:307:ILE:HD13	1:A:307:ILE:N	2.14	0.61
1:A:795:TYR:CE1	1:A:951:ARG:NH2	2.69	0.61
1:B:604:LEU:HG	1:B:648:LYS:HD2	1.83	0.60
1:A:545:THR:HG22	1:A:546:PRO:CD	2.29	0.60
1:A:99:ASP:O	1:A:217:LYS:NZ	2.32	0.59
1:B:236:ASP:OD2	1:B:239:GLN:HG2	2.02	0.59
1:A:600:LEU:O	1:A:600:LEU:HD23	2.02	0.59
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.85	0.59
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.84	0.59
1:A:894:LEU:HG	1:A:925:VAL:HG21	1.85	0.58
1:B:843:ILE:HG22	1:B:844:GLN:H	1.68	0.58
1:B:583:ALA:CB	1:B:626:GLY:HA2	2.33	0.58
1:A:776:TRP:HA	1:A:953:LYS:O	2.04	0.58
1:B:94:ILE:HG13	1:B:248:TYR:HB3	1.85	0.57
1:B:557:SER:HB2	1:B:742:MET:HE3	1.84	0.57
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.87	0.57
1:A:213:HIS:ND1	1:A:214:PRO:HD2	2.20	0.57
1:A:683:MET:HA	1:A:792:GLU:OE1	2.05	0.56
1:A:894:LEU:HD11	1:A:925:VAL:HG11	1.86	0.56
1:A:625:TYR:CZ	1:A:765:ARG:HG3	2.41	0.56
1:B:285:LEU:HD12	1:B:286:PRO:CD	2.33	0.56
1:B:565:ASP:OD1	1:B:566:LYS:HG3	2.07	0.55
1:A:473:PRO:O	1:A:476:VAL:HG12	2.06	0.55
1:A:643:LYS:HE3	1:A:647:GLU:OE1	2.07	0.55
1:B:392:LEU:O	1:B:396:GLN:HG3	2.06	0.55
1:B:787:ASN:HB2	1:B:961:ARG:HH21	1.71	0.54
1:A:306:PRO:HD3	1:A:481:VAL:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:ASN:C	1:A:960:ALA:HB2	2.27	0.54
1:A:864:GLU:OE2	1:A:951:ARG:NH2	2.25	0.54
1:A:927:TYR:CE1	1:A:931:LEU:HD21	2.43	0.54
1:B:229:ARG:HB3	1:B:230:PRO:HD3	1.89	0.54
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.89	0.54
1:B:152:ASP:OD1	1:B:431:ARG:HD3	2.08	0.54
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.43	0.53
1:A:411:PHE:HB2	1:A:459:PHE:CD1	2.43	0.53
1:B:507:ASP:HB3	1:B:511:LYS:NZ	2.23	0.53
1:A:206:LYS:HB3	1:A:216:SER:HA	1.88	0.53
1:A:817:GLU:HB3	1:A:818:PRO:HD3	1.90	0.53
1:A:446:LEU:N	1:A:446:LEU:HD12	2.23	0.53
1:B:473:PRO:O	1:B:476:VAL:HG12	2.09	0.53
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.44	0.53
1:A:114:LEU:HD13	1:A:168:PHE:HB3	1.91	0.53
1:A:460:ARG:HG3	1:A:460:ARG:NH1	2.23	0.53
1:A:810:LEU:HD23	1:A:936:ILE:HD11	1.92	0.52
1:B:153:VAL:CG2	1:B:154:SER:N	2.43	0.52
1:B:1009:LYS:HD3	1:B:1009:LYS:N	2.25	0.52
1:B:787:ASN:HB2	1:B:961:ARG:NH2	2.24	0.52
1:B:843:ILE:HG22	1:B:844:GLN:N	2.24	0.51
1:B:138:SER:HB2	1:B:150:TYR:O	2.10	0.51
1:B:213:HIS:ND1	1:B:214:PRO:HD2	2.25	0.51
1:B:227:GLU:O	1:B:230:PRO:HD2	2.11	0.51
1:B:796:GLN:HB3	1:B:952:HIS:HB2	1.92	0.51
1:B:75:VAL:HG22	1:B:256:VAL:HG22	1.92	0.51
1:A:538:LEU:HD13	1:A:734:THR:HG23	1.92	0.51
1:B:189:GLU:O	1:B:192:LYS:HB3	2.11	0.51
1:A:685:TYR:HB2	1:A:956:VAL:HG11	1.91	0.51
1:A:1011:HIS:O	1:A:1012:ILE:HB	2.10	0.51
1:B:538:LEU:H	1:B:732:ASN:HD21	1.59	0.51
1:B:799:MET:HE3	1:B:1008:VAL:CG2	2.34	0.51
1:B:246:SER:O	1:B:281:LYS:HE2	2.10	0.51
1:A:690:MET:O	1:A:768:GLU:HG3	2.11	0.51
1:B:246:SER:O	1:B:281:LYS:CE	2.59	0.51
1:A:305:VAL:HG22	1:A:485:PHE:HB2	1.93	0.50
1:B:192:LYS:HG3	1:B:677:GLN:OE1	2.12	0.50
1:A:406:PRO:HB3	1:A:459:PHE:CZ	2.47	0.50
1:A:365:GLU:H	1:A:365:GLU:CD	2.15	0.49
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.94	0.49
1:A:288:PHE:O	1:A:369:GLY:HA3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HB	1:B:41:PRO:HD2	1.95	0.49
1:A:689:LEU:CD2	1:A:995:MET:HG2	2.43	0.49
1:A:460:ARG:HG3	1:A:460:ARG:HH11	1.78	0.49
1:B:620:LEU:HD13	1:B:629:LEU:HD13	1.94	0.49
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.48	0.49
1:A:49:ARG:HG2	1:A:50:ILE:N	2.28	0.49
1:A:574:LEU:CD2	1:A:729:LEU:HD22	2.40	0.49
1:A:759:LEU:HB2	1:A:762:GLN:HG3	1.95	0.49
1:A:251:SER:OG	1:A:280:ASN:HB2	2.13	0.48
1:A:324:LYS:HE3	1:A:325:TYR:CE1	2.48	0.48
1:A:842:GLY:C	1:A:843:ILE:HD13	2.34	0.48
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.95	0.48
1:B:894:LEU:HG	1:B:925:VAL:HG21	1.96	0.48
1:A:346:LEU:HA	1:A:522:PHE:CE1	2.49	0.48
1:A:577:GLU:HG2	1:A:908:TRP:HZ2	1.77	0.48
1:A:995:MET:O	1:A:999:LYS:HG3	2.13	0.48
1:A:411:PHE:HB2	1:A:459:PHE:CE1	2.48	0.48
1:B:71:ASN:HB2	1:B:251:SER:OG	2.14	0.48
1:A:600:LEU:HD23	1:A:600:LEU:C	2.35	0.48
1:A:599:LEU:HD23	1:A:662:ILE:HD12	1.96	0.47
1:B:152:ASP:OD1	1:B:431:ARG:CD	2.62	0.47
1:B:793:ILE:O	1:B:847:ARG:HA	2.14	0.47
1:A:67:LEU:N	1:A:446:LEU:HD23	2.29	0.47
1:A:433:TYR:CE1	1:A:437:ILE:HD11	2.50	0.47
1:B:716:ILE:HB	1:B:717:PRO:CD	2.32	0.47
1:A:406:PRO:CB	1:A:459:PHE:CE2	2.97	0.47
1:B:201:LEU:HD23	1:B:201:LEU:HA	1.65	0.47
1:A:559:LEU:HD22	1:A:742:MET:HB2	1.96	0.47
1:B:199:TRP:CE2	4:B:1105:DIO:H2'1	2.50	0.47
1:B:979:ASN:HB3	1:B:980:LEU:H	1.36	0.47
1:A:367:ALA:HB3	1:A:370:PHE:CE1	2.50	0.47
1:A:822:THR:O	1:A:827:GLU:HG3	2.15	0.47
1:A:882:PHE:CE2	1:A:886:ILE:HD11	2.50	0.47
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.97	0.47
1:A:76:LEU:HD23	1:A:437:ILE:HG21	1.96	0.47
1:A:577:GLU:HG2	1:A:908:TRP:CZ2	2.50	0.47
1:A:73:ILE:HG13	1:A:251:SER:HB2	1.96	0.46
1:B:108:HIS:O	1:B:111:GLU:HB3	2.15	0.46
1:B:245:HIS:O	1:B:249:TYR:HB2	2.15	0.46
1:B:291:HIS:ND1	1:B:292:PRO:HD2	2.30	0.46
1:A:64:TYR:CE2	1:A:450:LEU:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:HIS:O	1:A:683:MET:HG3	2.16	0.46
1:A:925:VAL:O	1:A:928:LEU:HB3	2.14	0.46
1:A:121:TYR:HB3	1:A:126:GLU:HG2	1.97	0.46
1:A:458:GLU:O	1:A:459:PHE:C	2.53	0.46
1:A:680:GLN:OE1	1:A:680:GLN:HA	2.14	0.46
1:B:914:GLN:HA	1:B:916:TYR:CE2	2.50	0.46
1:B:227:GLU:C	1:B:230:PRO:HD2	2.36	0.46
1:B:359:LEU:HD23	1:B:360:VAL:N	2.31	0.46
1:A:793:ILE:O	1:A:847:ARG:HA	2.16	0.46
1:B:600:LEU:CD2	1:B:604:LEU:HD12	2.46	0.46
1:B:808:LEU:HD21	1:B:845:GLY:O	2.15	0.46
1:A:618:TYR:HA	1:A:630:SER:O	2.16	0.46
1:B:206:LYS:HG2	1:B:215:PHE:O	2.16	0.46
1:B:946:VAL:HA	1:B:951:ARG:NH1	2.31	0.46
1:B:85:LYS:HA	1:B:153:VAL:O	2.15	0.45
1:A:460:ARG:N	1:A:461:PRO:CD	2.79	0.45
1:A:865:ALA:O	1:A:869:THR:HG23	2.16	0.45
1:B:441:LEU:CD2	1:B:449:VAL:HG11	2.47	0.45
1:A:815:ILE:HG22	1:A:870:MET:CE	2.42	0.45
1:B:538:LEU:HD13	1:B:734:THR:HG23	1.99	0.45
1:B:771:LEU:HB2	1:B:952:HIS:HB3	1.98	0.45
1:A:73:ILE:HG12	1:A:254:MET:HB2	1.98	0.45
1:A:108:HIS:O	1:A:111:GLU:HB3	2.16	0.45
1:A:137:SER:OG	1:A:431:ARG:NH2	2.46	0.45
1:A:896:LYS:O	1:A:898:LYS:HD3	2.17	0.45
1:A:634:TYR:C	1:A:636:ASP:H	2.20	0.45
1:B:483:LYS:O	1:B:486:GLU:HB3	2.17	0.45
1:B:599:LEU:HD21	1:B:659:PHE:HA	1.99	0.45
1:A:946:VAL:HA	1:A:951:ARG:NH1	2.31	0.45
1:B:350:LEU:HB3	1:B:356:VAL:HG22	1.99	0.45
1:A:155:HIS:CE1	1:A:156:GLU:HG3	2.52	0.45
1:A:548:PRO:HG3	1:A:907:TYR:CD2	2.52	0.45
1:B:77:LEU:HD21	1:B:271:VAL:HG21	1.99	0.45
1:B:616:LEU:HD11	1:B:638:GLN:HG2	1.99	0.45
1:A:459:PHE:HB3	1:A:461:PRO:HD3	1.99	0.44
1:B:451:THR:HB	1:B:455:LEU:HD12	1.99	0.44
1:A:343:PRO:HG3	1:A:606:GLU:OE1	2.17	0.44
1:A:71:ASN:HB2	1:A:251:SER:OG	2.17	0.44
1:B:197:ASP:HA	1:B:200:ARG:HD3	1.99	0.44
1:A:460:ARG:HA	1:A:460:ARG:HD2	1.58	0.44
1:B:111:GLU:OE2	1:B:140:ALA:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ARG:HG2	1:A:756:LYS:HB2	1.99	0.44
1:B:374:ILE:HD12	1:B:376:ASN:ND2	2.33	0.44
1:A:422:PHE:CZ	1:A:451:THR:HG22	2.52	0.44
1:A:843:ILE:HD13	1:A:843:ILE:N	2.31	0.44
1:B:716:ILE:CB	1:B:717:PRO:CD	2.93	0.44
1:B:557:SER:HA	1:B:725:ILE:O	2.17	0.44
1:B:127:TYR:HE2	1:B:138:SER:HG	1.66	0.44
1:A:570:PRO:C	1:A:635:ASN:OD1	2.57	0.43
1:B:291:HIS:CE1	1:B:318:PRO:HB3	2.53	0.43
1:A:90:LEU:HD12	1:A:256:VAL:CG2	2.47	0.43
1:A:345:SER:OG	1:A:348:SER:HB3	2.19	0.43
1:A:601:LYS:HD3	1:A:620:LEU:HB3	2.00	0.43
1:A:66:GLY:O	1:A:67:LEU:HB3	2.17	0.43
1:A:334:LEU:HD23	1:A:334:LEU:HA	1.83	0.43
1:A:323:GLN:O	1:A:326:TYR:HB3	2.18	0.43
1:A:795:TYR:CE1	1:A:953:LYS:HD2	2.53	0.43
1:B:583:ALA:HB2	1:B:626:GLY:HA2	1.99	0.43
1:A:604:LEU:HD23	1:A:604:LEU:HA	1.76	0.43
1:A:882:PHE:CE1	1:A:933:LYS:HA	2.54	0.43
1:B:594:TYR:CE2	1:B:598:GLU:HG3	2.54	0.43
1:A:575:ASN:O	1:A:727:ALA:HA	2.18	0.43
1:B:93:HIS:CD2	1:B:93:HIS:O	2.71	0.42
1:A:912:ILE:HG13	1:A:913:SER:N	2.33	0.42
1:A:328:SER:O	1:A:329:ASN:CB	2.67	0.42
1:A:689:LEU:HD23	1:A:995:MET:HG2	2.00	0.42
1:B:586:ASP:HB2	1:B:587:PRO:HD2	2.01	0.42
1:A:49:ARG:CG	1:A:50:ILE:N	2.83	0.42
1:A:411:PHE:CB	1:A:459:PHE:CD1	3.03	0.42
1:A:430:PRO:O	1:A:434:THR:HG23	2.19	0.42
1:A:460:ARG:HH11	1:A:460:ARG:CG	2.32	0.42
1:B:548:PRO:HG3	1:B:907:TYR:CD2	2.54	0.42
1:A:262:GLU:HB2	1:A:267:LEU:HD21	2.02	0.42
1:A:318:PRO:HD2	1:A:475:ASN:O	2.20	0.42
1:A:406:PRO:HB3	1:A:459:PHE:CE2	2.55	0.42
1:B:139:ASN:HB3	1:B:150:TYR:CZ	2.55	0.42
1:A:175:ASP:OD1	1:A:177:SER:HB3	2.19	0.42
1:B:620:LEU:HA	1:B:620:LEU:HD12	1.78	0.42
1:A:359:LEU:C	1:A:359:LEU:HD23	2.40	0.42
1:A:586:ASP:HA	1:A:695:TRP:CZ2	2.55	0.42
1:A:597:LEU:HD11	1:A:627:MET:HG2	2.01	0.42
1:B:90:LEU:HD12	1:B:256:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:872:LYS:HD2	1:B:872:LYS:HA	1.81	0.42
1:A:838:ARG:O	1:A:839:ARG:HD2	2.20	0.41
1:B:74:LYS:O	1:B:255:ALA:HA	2.20	0.41
1:A:285:LEU:HA	1:A:285:LEU:HD12	1.71	0.41
1:A:545:THR:HG23	1:A:546:PRO:HD2	1.98	0.41
1:B:683:MET:HA	1:B:792:GLU:OE1	2.20	0.41
1:B:714:ALA:O	1:B:717:PRO:HD2	2.20	0.41
1:B:774:ARG:HD2	1:B:949:PRO:HA	2.01	0.41
1:B:776:TRP:HA	1:B:953:LYS:O	2.20	0.41
1:B:526:THR:O	1:B:527:LYS:C	2.58	0.41
1:B:777:PHE:HA	1:B:990:GLU:O	2.21	0.41
1:A:123:LYS:HE2	1:A:126:GLU:OE1	2.20	0.41
1:A:542:LYS:HA	1:A:542:LYS:HD2	1.83	0.41
1:A:913:SER:HB2	5:A:1106:EPE:H101	2.02	0.41
1:A:197:ASP:OD1	1:A:306:PRO:CA	2.69	0.41
1:A:770:GLN:O	1:A:1003:PRO:HD2	2.21	0.41
1:A:172:PRO:HG2	1:A:174:PHE:CE2	2.56	0.41
1:A:599:LEU:HD21	1:A:659:PHE:HA	2.01	0.41
1:B:88:ALA:HA	1:B:257:VAL:O	2.20	0.41
1:A:214:PRO:O	1:A:217:LYS:HG3	2.20	0.41
1:A:306:PRO:CG	1:A:481:VAL:CG1	2.95	0.41
1:B:164:ARG:HG3	1:B:164:ARG:HH11	1.85	0.41
1:A:684:TYR:OH	1:A:697:LYS:HG2	2.21	0.41
1:B:942:GLU:O	1:B:948:ALA:HB1	2.21	0.41
1:B:961:ARG:HE	1:B:961:ARG:HB3	1.74	0.41
1:A:44:ASN:HA	1:A:45:PRO:HD3	1.91	0.41
1:A:333:TYR:CE2	1:A:459:PHE:CE1	3.08	0.41
1:A:963:MET:HG2	1:A:964:ASP:N	2.32	0.41
1:B:299:LYS:HD2	1:B:510:ILE:HG13	2.03	0.41
1:A:111:GLU:OE2	1:A:140:ALA:CB	2.65	0.41
1:A:418:ASN:HB3	1:A:454:TYR:O	2.21	0.41
1:A:843:ILE:HG22	1:A:844:GLN:N	2.36	0.41
1:B:820:PHE:CZ	1:B:824:ARG:HD3	2.56	0.41
1:A:787:ASN:HA	1:A:960:ALA:HB1	2.02	0.40
1:B:293:PHE:CE2	1:B:372:PHE:HE2	2.39	0.40
1:A:299:LYS:HD2	1:A:510:ILE:HG13	2.01	0.40
1:A:569:LEU:HA	1:A:569:LEU:HD23	1.77	0.40
1:B:722:ARG:HB3	1:B:758:LEU:HD23	2.03	0.40
1:A:257:VAL:HG21	1:A:437:ILE:HG22	2.03	0.40
1:B:311:ARG:HA	1:B:481:VAL:O	2.22	0.40
1:B:635:ASN:O	1:B:636:ASP:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:ALA:O	1:A:951:ARG:HD2	2.22	0.40
1:B:868:ILE:HD11	1:B:984:PRO:HG3	2.02	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	953/990 (96%)	920 (96%)	33 (4%)	0	100	100
1	B	954/990 (96%)	915 (96%)	39 (4%)	0	100	100
All	All	1907/1980 (96%)	1835 (96%)	72 (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	853/879 (97%)	849 (100%)	4 (0%)	88	96
1	B	853/879 (97%)	852 (100%)	1 (0%)	93	98
All	All	1706/1758 (97%)	1701 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	457	GLU
1	A	460	ARG
1	A	756	LYS
1	B	774	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
4	DIO	A	1104	-	6,6,6	0.71	0	6,6,6	1.45	2 (33%)
4	DIO	B	1104	-	6,6,6	0.75	0	6,6,6	0.93	0
5	EPE	A	1106	-	15,15,15	0.88	1 (6%)	18,20,20	1.90	5 (27%)
5	EPE	B	1106	-	15,15,15	1.18	1 (6%)	18,20,20	1.91	4 (22%)
4	DIO	A	1105	-	6,6,6	0.74	0	6,6,6	0.86	0
3	VQD	A	1102	2	41,42,42	2.80	9 (21%)	47,59,59	1.85	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DIO	B	1105	-	6,6,6	0.74	0	6,6,6	0.86	0
4	DIO	B	1103	-	6,6,6	0.68	0	6,6,6	0.74	0
4	DIO	A	1103	-	6,6,6	0.66	0	6,6,6	0.71	0
3	VQD	B	1102	2	41,42,42	2.72	8 (19%)	47,59,59	1.58	7 (14%)

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
4	DIO	A	1104	-	-	-	0/1/1/1
4	DIO	B	1104	-	-	-	0/1/1/1
5	EPE	A	1106	-	-	7/9/19/19	0/1/1/1
5	EPE	B	1106	-	-	5/9/19/19	0/1/1/1
4	DIO	A	1105	-	-	-	0/1/1/1
3	VQD	A	1102	2	-	2/18/37/37	0/5/5/5
4	DIO	B	1105	-	-	-	0/1/1/1
4	DIO	B	1103	-	-	-	0/1/1/1
4	DIO	A	1103	-	-	-	0/1/1/1
3	VQD	B	1102	2	-	2/18/37/37	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	VQD	C03-N02	13.65	1.47	1.32
3	B	1102	VQD	C03-N02	13.64	1.47	1.32
3	B	1102	VQD	C18-C19	5.59	1.44	1.36
3	A	1102	VQD	C20-N25	-5.30	1.42	1.47
3	A	1102	VQD	C18-C19	4.83	1.43	1.36
3	B	1102	VQD	C20-N25	-4.71	1.42	1.47
3	A	1102	VQD	C26-N25	4.69	1.45	1.34
5	B	1106	EPE	C10-S	4.26	1.83	1.77
3	B	1102	VQD	C26-N25	4.03	1.44	1.34
3	A	1102	VQD	C05-N17	-3.42	1.44	1.49
5	A	1106	EPE	C10-S	2.87	1.81	1.77
3	A	1102	VQD	O38-C03	-2.66	1.17	1.23
3	A	1102	VQD	C18-N17	-2.40	1.33	1.35
3	B	1102	VQD	C24-N25	-2.35	1.42	1.47
3	B	1102	VQD	C05-N17	-2.27	1.45	1.49
3	A	1102	VQD	C27-C26	2.24	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	VQD	C24-N25	-2.16	1.43	1.47
3	B	1102	VQD	O38-C03	-2.16	1.18	1.23
3	B	1102	VQD	C27-C26	2.07	1.53	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1102	VQD	C23-O22-C21	6.53	119.02	109.97
3	B	1102	VQD	C23-O22-C21	5.03	116.94	109.97
3	A	1102	VQD	O01-N02-C03	4.39	126.28	119.79
5	B	1106	EPE	C5-N4-C3	4.15	118.17	108.83
5	A	1106	EPE	C5-N4-C3	4.03	117.89	108.83
3	B	1102	VQD	O01-N02-C03	3.91	125.57	119.79
5	A	1106	EPE	O1S-S-C10	3.84	111.54	106.92
3	A	1102	VQD	C20-C19-N36	3.62	125.58	120.23
3	A	1102	VQD	O38-C03-C04	-3.48	116.40	121.50
3	B	1102	VQD	C20-C19-N36	3.44	125.31	120.23
3	A	1102	VQD	C04-C03-N02	3.44	120.35	115.14
5	A	1106	EPE	C7-N4-C5	3.22	119.47	111.23
5	A	1106	EPE	C6-N1-C2	3.19	116.01	108.83
5	B	1106	EPE	O3S-S-C10	3.12	110.81	105.77
3	A	1102	VQD	O22-C23-C24	3.11	118.64	111.80
5	A	1106	EPE	C7-N4-C3	2.95	118.78	111.23
3	B	1102	VQD	C04-C03-N02	2.85	119.46	115.14
5	B	1106	EPE	O1S-S-C10	2.83	110.33	106.92
3	B	1102	VQD	C18-C19-N36	-2.79	106.20	110.14
5	B	1106	EPE	O2S-S-C10	2.78	110.26	106.92
4	A	1104	DIO	C2'-O1'-C1'	2.52	118.30	109.89
3	B	1102	VQD	C23-C24-N25	-2.36	107.09	109.36
3	A	1102	VQD	C21-C20-C19	2.24	116.47	110.83
3	A	1102	VQD	O35-C26-N25	-2.17	118.07	121.59
4	A	1104	DIO	O1'-C2'-C2	2.08	121.11	110.95
3	A	1102	VQD	C18-N17-C05	-2.05	123.67	125.48
3	B	1102	VQD	C28-C27-C34	2.02	121.63	119.24

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	VQD	C03-C04-C05-C06
3	A	1102	VQD	C03-C04-C05-N17
3	B	1102	VQD	C03-C04-C05-C06

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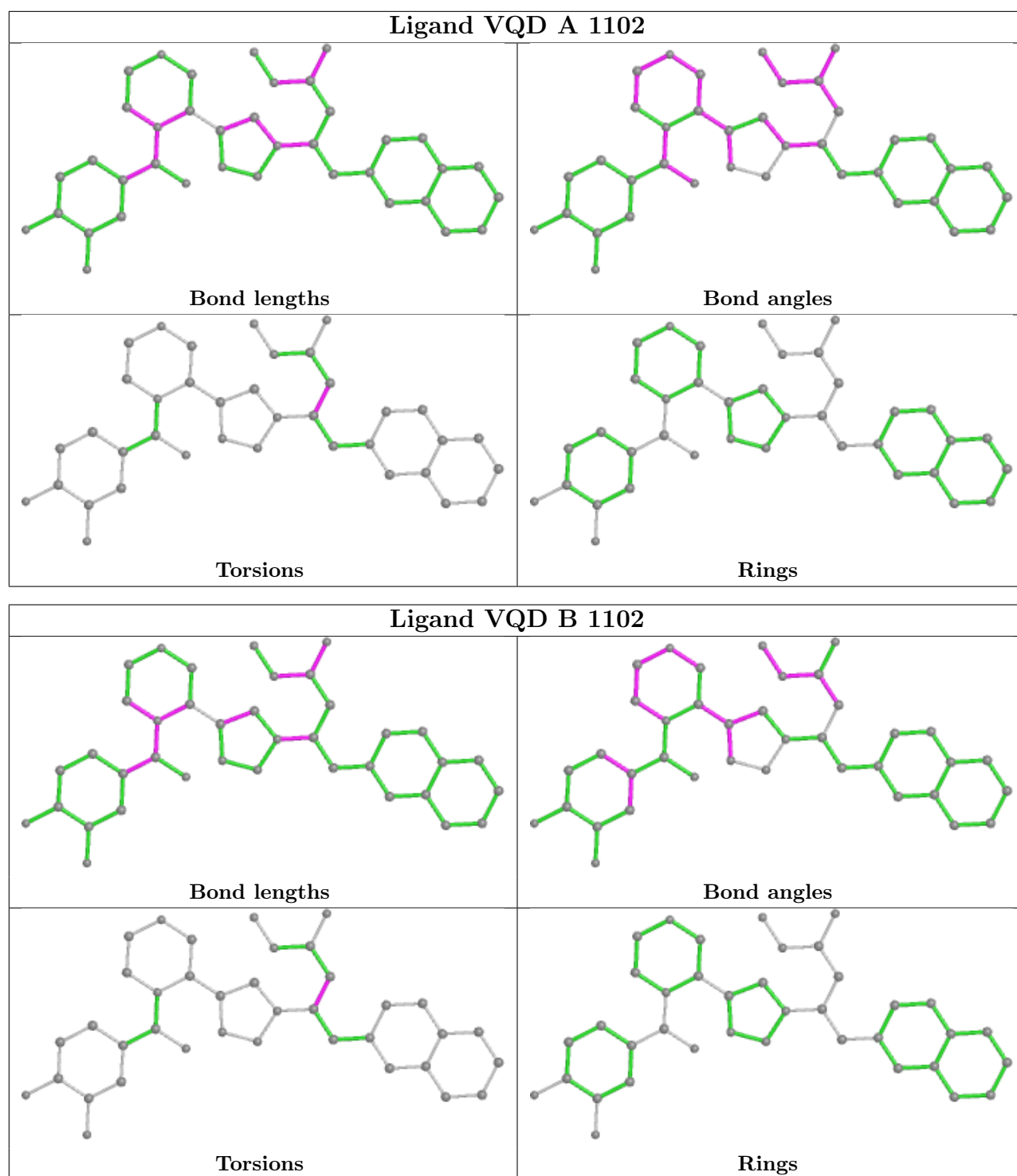
Mol	Chain	Res	Type	Atoms
3	B	1102	VQD	C03-C04-C05-N17
5	A	1106	EPE	C9-C10-S-O1S
5	A	1106	EPE	C9-C10-S-O2S
5	A	1106	EPE	C9-C10-S-O3S
5	B	1106	EPE	C9-C10-S-O2S
5	B	1106	EPE	C9-C10-S-O3S
5	A	1106	EPE	N4-C7-C8-O8
5	A	1106	EPE	C10-C9-N1-C2
5	B	1106	EPE	C10-C9-N1-C2
5	B	1106	EPE	C10-C9-N1-C6
5	B	1106	EPE	C9-C10-S-O1S
5	A	1106	EPE	S-C10-C9-N1
5	A	1106	EPE	C10-C9-N1-C6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1106	EPE	1	0
4	B	1105	DIO	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 ⓘ

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	957/990 (96%)	-0.48	1 (0%) 95 89	30, 53, 76, 115	0
1	B	958/990 (96%)	-0.53	1 (0%) 95 89	27, 45, 70, 127	0
All	All	1915/1980 (96%)	-0.50	2 (0%) 95 89	27, 49, 74, 127	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	GLY	2.3
1	A	52	ASN	2.2

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 monosaccharides 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
4	DIO	A	1104	6/6	0.74	0.31	71,91,129,129	0
4	DIO	A	1103	6/6	0.78	0.36	81,97,120,120	0
4	DIO	B	1103	6/6	0.80	0.39	75,102,120,120	0

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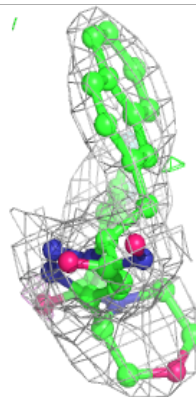
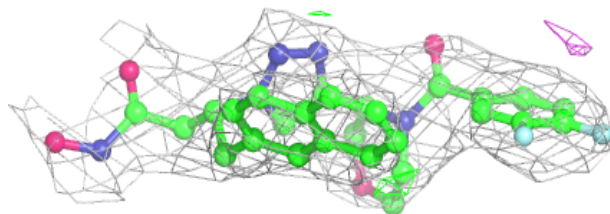
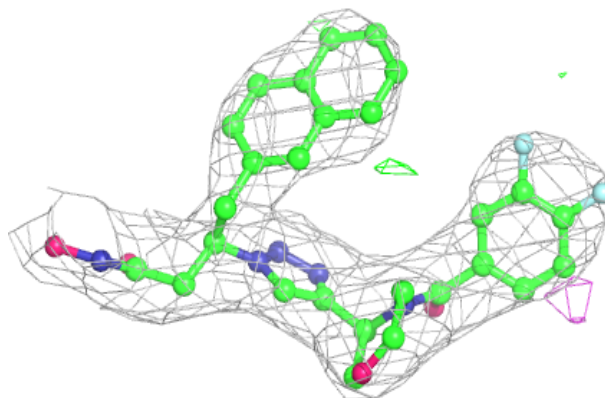
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DIO	A	1105	6/6	0.82	0.26	65,88,129,129	0
4	DIO	B	1104	6/6	0.83	0.33	57,80,117,117	0
4	DIO	B	1105	6/6	0.86	0.30	51,65,120,120	0
5	EPE	A	1106	15/15	0.94	0.18	54,90,108,108	0
5	EPE	B	1106	15/15	0.94	0.22	54,79,103,109	0
3	VQD	A	1102	38/38	0.96	0.19	41,54,72,73	0
3	VQD	B	1102	38/38	0.96	0.17	41,49,62,76	0
2	ZN	A	1101	1/1	0.99	0.12	52,52,52,52	0
2	ZN	B	1101	1/1	0.99	0.17	42,42,42,42	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.

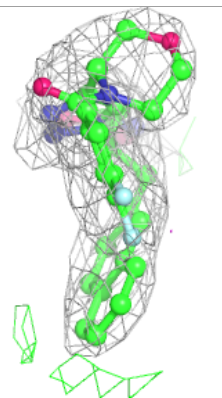
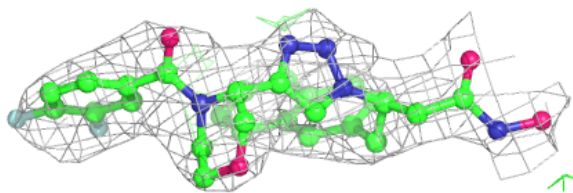
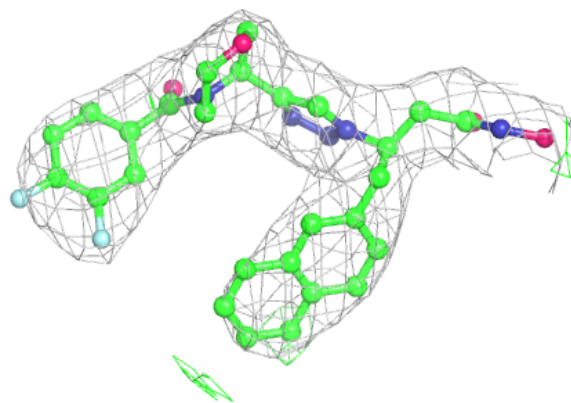
Electron density around VQD A 1102:

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 VQD B 1102:

$2mF_o-DF_c$ (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.