



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:52 PM UTC

PDB ID : 2G49 / pdb_00002g49
Title : Crystal structure of human insulin-degrading enzyme in complex with glucagon
Authors : Shen, Y.; Tang, W.-J.
Deposited on : 2006-02-21
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

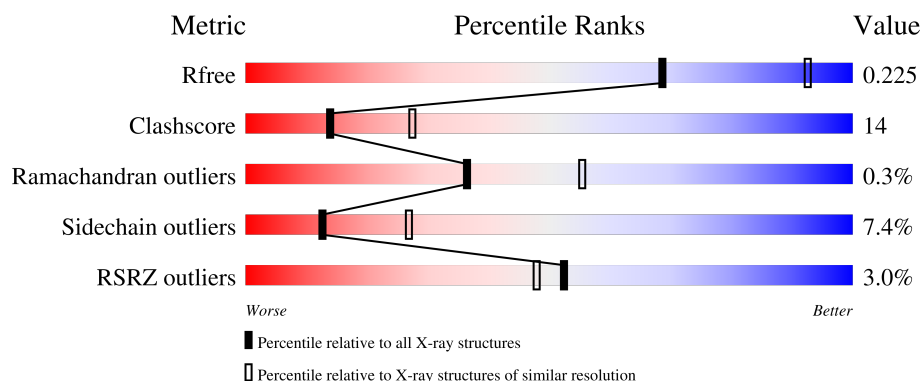
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	2% 69% 25% • •
1	B	990	3% 67% 25% 5% •
2	C	29	28% 17% 14% 7% 62%
2	D	29	21% 10% 14% 7% 69%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16638 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	970	Total	C	N	O	S	0	0	0
			7889	5073	1327	1455	34			
1	B	966	Total	C	N	O	S	0	0	0
			7866	5064	1320	1448	34			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	UNP Q5T5N2
A	31	HIS	-	expression tag	UNP Q5T5N2
A	32	HIS	-	expression tag	UNP Q5T5N2
A	33	HIS	-	expression tag	UNP Q5T5N2
A	34	HIS	-	expression tag	UNP Q5T5N2
A	35	HIS	-	expression tag	UNP Q5T5N2
A	36	HIS	-	expression tag	UNP Q5T5N2
A	37	ALA	-	cloning artifact	UNP Q5T5N2
A	38	ALA	-	cloning artifact	UNP Q5T5N2
A	39	GLY	-	cloning artifact	UNP Q5T5N2
A	40	ILE	-	cloning artifact	UNP Q5T5N2
A	41	PRO	-	cloning artifact	UNP Q5T5N2
A	111	GLN	GLU	engineered mutation	UNP Q5T5N2
B	30	MET	-	initiating methionine	UNP Q5T5N2
B	31	HIS	-	expression tag	UNP Q5T5N2
B	32	HIS	-	expression tag	UNP Q5T5N2
B	33	HIS	-	expression tag	UNP Q5T5N2
B	34	HIS	-	expression tag	UNP Q5T5N2
B	35	HIS	-	expression tag	UNP Q5T5N2
B	36	HIS	-	expression tag	UNP Q5T5N2
B	37	ALA	-	cloning artifact	UNP Q5T5N2
B	38	ALA	-	cloning artifact	UNP Q5T5N2
B	39	GLY	-	cloning artifact	UNP Q5T5N2
B	40	ILE	-	cloning artifact	UNP Q5T5N2
B	41	PRO	-	cloning artifact	UNP Q5T5N2

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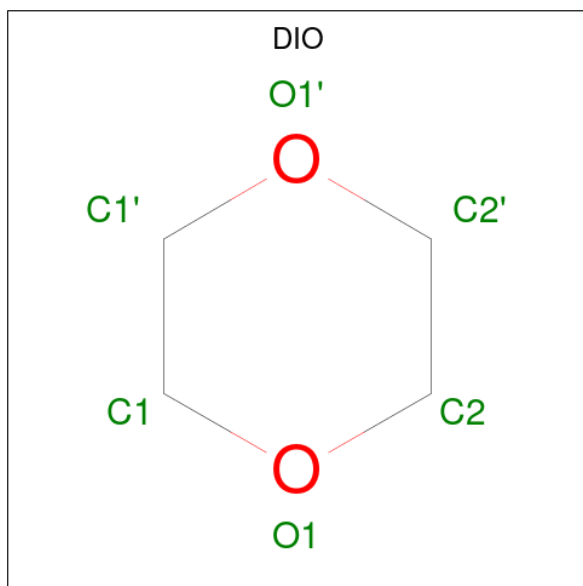
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Chain	Residue	Modelled	Actual	Comment	Reference
B	111	GLN	GLU	engineered mutation	UNP Q5T5N2

- Molecule 2 is a protein called glucagon preproprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total 94	C 61	N 17	O 15	S 1	0	0	0
2	D	9	Total 82	C 55	N 14	O 12	S 1	0	0	0

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	401	Total	O	0	0
			401	401		
4	B	292	Total	O	0	0
			292	292		

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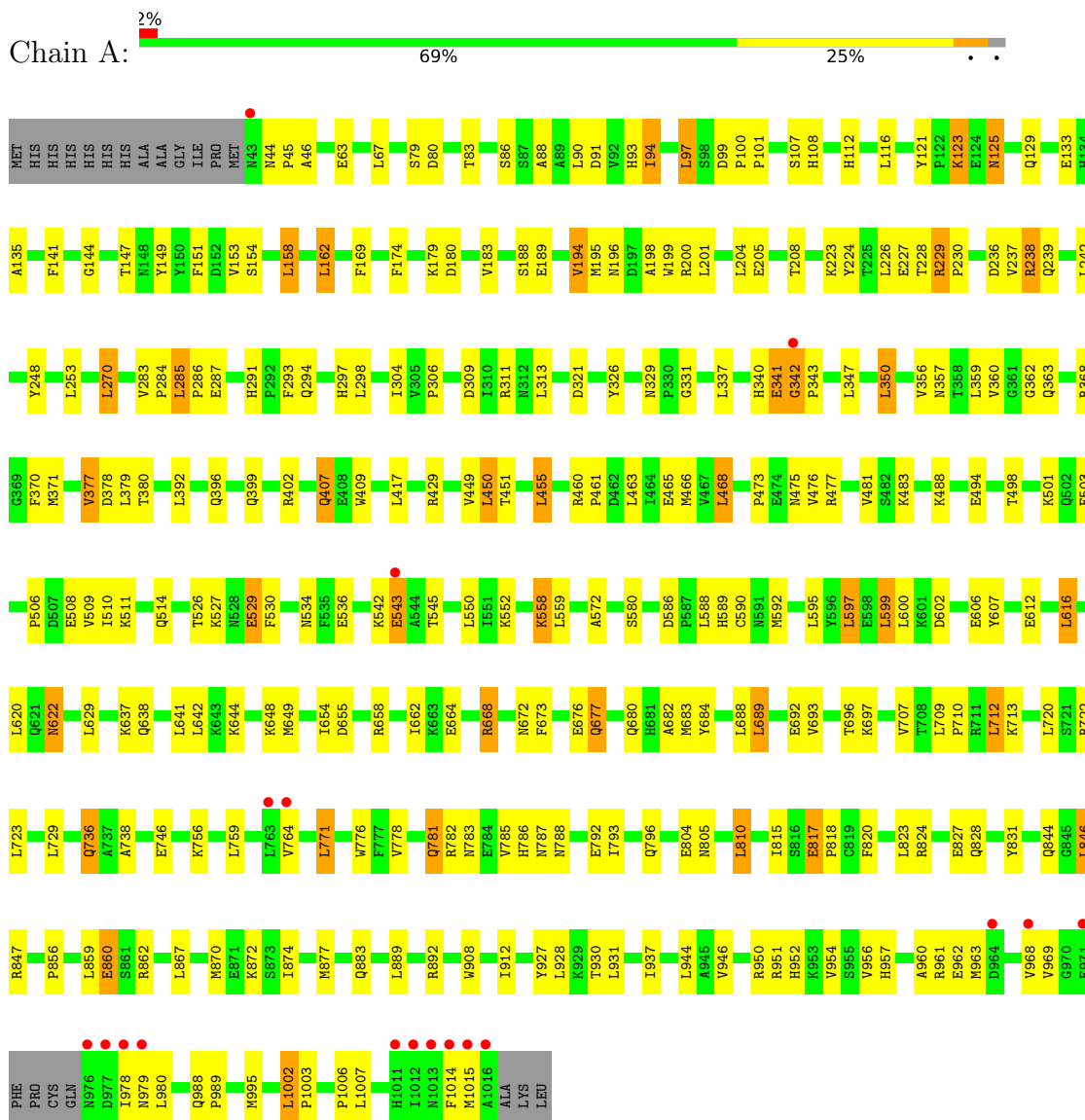
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	O	0	0
			2	2		

3 Residue-property plots

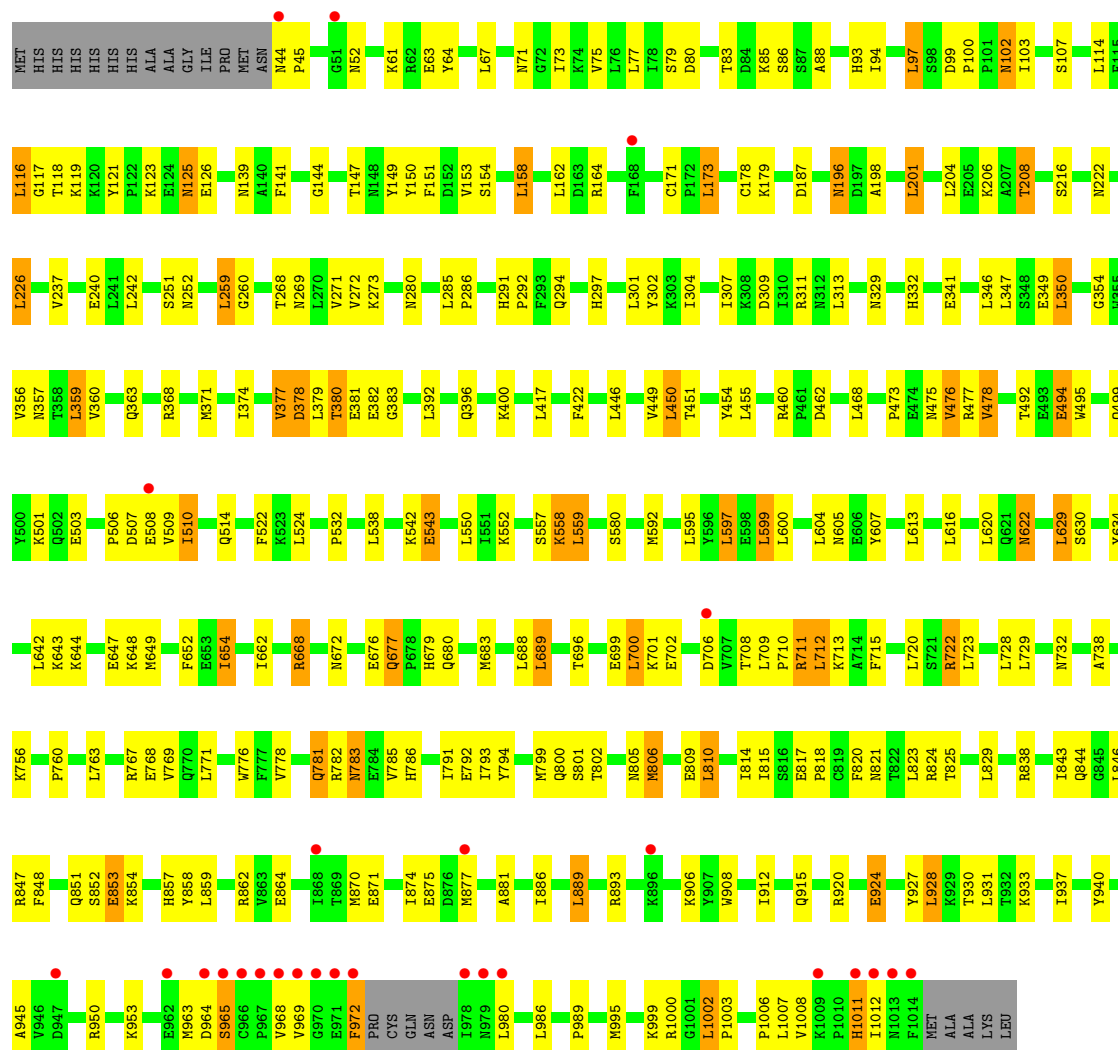
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Insulin-degrading enzyme

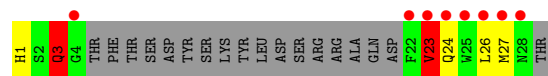


• Molecule 1: Insulin-degrading enzyme

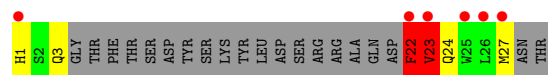




• Molecule 2: glucagon preproprotein



• Molecule 2: glucagon preproprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	262.72Å 262.72Å 90.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.80 – 2.50 29.80 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.80-2.50) 97.0 (29.80-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.225 0.197 , 0.225	Depositor DCC
R_{free} test set	12309 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16638	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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: DIO

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	0.43	0/8085	0.92	20/10938 (0.2%)
1	B	0.40	0/8063	0.89	19/10907 (0.2%)
2	C	1.63	2/96 (2.1%)	1.52	3/127 (2.4%)
2	D	1.39	1/84 (1.2%)	0.91	0/111
All	All	0.44	3/16328 (0.0%)	0.91	42/22083 (0.2%)

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
2	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	23	VAL	CA-C	-5.86	1.45	1.52
2	D	24	GLN	N-CA	-5.51	1.39	1.46
2	C	23	VAL	CA-CB	-5.45	1.45	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	TYR	CA-C-N	9.30	129.37	119.05
1	A	121	TYR	C-N-CA	9.30	129.37	119.05
1	A	494	GLU	N-CA-C	8.03	120.03	111.28
1	B	341	GLU	N-CA-C	-7.96	97.30	109.95
1	B	495	TRP	N-CA-C	7.78	120.85	111.82
1	A	341	GLU	N-CA-C	-7.32	98.23	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	LEU	N-CA-C	7.21	119.85	108.67
1	B	116	LEU	N-CA-C	6.91	120.67	112.93
1	B	963	MET	N-CA-C	-6.57	97.71	108.41
1	A	545	THR	CA-C-N	6.55	126.14	119.19
1	A	545	THR	C-N-CA	6.55	126.14	119.19
1	B	121	TYR	CA-C-N	6.36	126.11	119.05
1	B	121	TYR	C-N-CA	6.36	126.11	119.05
2	C	23	VAL	CA-C-N	-6.26	112.97	122.81
2	C	23	VAL	C-N-CA	-6.26	112.97	122.81
1	A	677	GLN	CA-C-N	6.26	125.75	119.24
1	A	677	GLN	C-N-CA	6.26	125.75	119.24
1	A	1014	PHE	N-CA-C	6.26	120.47	109.96
1	A	380	THR	N-CA-C	-6.23	101.75	110.35
1	B	677	GLN	CA-C-N	6.05	125.53	119.24
1	B	677	GLN	C-N-CA	6.05	125.53	119.24
1	A	944	LEU	N-CA-C	5.88	120.96	113.55
1	B	605	ASN	N-CA-C	5.62	117.85	111.11
1	B	449	VAL	N-CA-C	5.58	116.98	110.62
1	A	429	ARG	N-CA-C	-5.56	103.04	109.93
1	A	342	GLY	CA-C-N	5.47	126.68	119.84
1	A	342	GLY	C-N-CA	5.47	126.68	119.84
1	A	116	LEU	N-CA-C	5.44	119.46	113.21
1	B	307	ILE	N-CA-C	-5.32	105.66	110.82
1	B	476	VAL	N-CA-C	5.31	117.20	108.97
1	B	1011	HIS	N-CA-C	-5.29	102.64	110.46
1	A	590	CYS	N-CA-C	-5.28	105.60	111.36
2	C	3	GLN	N-CA-C	5.27	118.21	110.30
1	B	654	ILE	N-CA-C	5.27	115.89	109.30
1	A	194	VAL	N-CA-C	5.24	116.60	110.62
1	B	559	LEU	N-CA-C	5.20	116.88	108.41
1	B	1012	ILE	N-CA-C	5.19	116.76	108.87
1	B	953	LYS	N-CA-C	5.11	117.82	109.59
1	A	341	GLU	CA-C-N	-5.10	113.87	121.87
1	A	341	GLU	C-N-CA	-5.10	113.87	121.87
1	B	557	SER	N-CA-C	5.09	116.80	108.76
1	B	853	GLU	N-CA-C	-5.06	106.62	112.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	22	PHE	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	7889	0	7792	210	0
1	B	7866	0	7776	247	0
2	C	94	0	86	8	0
2	D	82	0	77	4	0
3	A	6	0	8	2	0
3	B	6	0	8	0	0
4	A	401	0	0	9	0
4	B	292	0	0	10	0
4	C	2	0	0	0	0
All	All	16638	0	15747	455	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 14.

All (455) 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:116:LEU:HD23	1:B:178:CYS:HB3	1.35	1.06
1:B:208:THR:HG23	1:B:477:ARG:HH22	1.14	1.06
1:B:782:ARG:HH21	1:B:964:ASP:HA	1.21	1.01
1:B:356:VAL:HG11	1:B:377:VAL:HG22	1.48	0.95
1:A:764:VAL:HA	1:B:1000:ARG:HH22	1.38	0.88
1:B:309:ASP:H	1:B:672:ASN:HD21	1.18	0.87
1:B:782:ARG:NH2	1:B:964:ASP:HA	1.91	0.85
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.21	0.85
1:A:764:VAL:HA	1:B:1000:ARG:NH2	1.93	0.83
1:B:778:VAL:HG11	1:B:968:VAL:HG13	1.61	0.81
1:A:550:LEU:HD11	1:A:558:LYS:HG3	1.60	0.81
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.30	0.80
1:A:309:ASP:H	1:A:672:ASN:HD21	1.30	0.79
1:B:368:ARG:HD2	4:B:2098:HOH:O	1.82	0.79
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.84	0.77
1:B:864:GLU:HG2	1:B:986:LEU:HD21	1.66	0.77
1:B:102:ASN:HD22	1:B:102:ASN:H	1.31	0.77
1:B:356:VAL:CG1	1:B:377:VAL:HG22	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:OE1	2:C:24:GLN:HB3	1.87	0.75
1:A:196:ASN:HD22	1:A:199:TRP:H	1.34	0.74
1:B:208:THR:CG2	1:B:477:ARG:HH22	1.96	0.74
1:B:805:ASN:ND2	1:B:844:GLN:HE22	1.84	0.74
1:A:123:LYS:HD2	1:A:125:ASN:ND2	2.02	0.74
1:A:599:LEU:HD13	1:A:662:ILE:HD12	1.70	0.73
1:A:125:ASN:H	1:A:125:ASN:HD22	1.35	0.73
1:B:309:ASP:H	1:B:672:ASN:ND2	1.87	0.72
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.25	0.72
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.36	0.72
1:A:872:LYS:HE2	4:A:2044:HOH:O	1.89	0.72
1:A:783:ASN:ND2	1:A:786:HIS:H	1.88	0.72
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.72	0.71
1:B:908:TRP:CZ2	1:B:912:ILE:HD11	2.24	0.71
1:B:354:GLY:O	1:B:380:THR:HG21	1.90	0.70
1:B:119:LYS:HD3	1:B:171:CYS:HB2	1.73	0.70
1:A:194:VAL:HG12	1:A:195:MET:HE3	1.73	0.70
1:A:477:ARG:HB3	1:A:477:ARG:HH11	1.55	0.70
1:B:357:ASN:HB2	1:B:378:ASP:OD2	1.91	0.70
1:B:969:VAL:HG21	1:B:989:PRO:HD3	1.74	0.70
1:A:815:ILE:HG22	1:A:870:MET:HE2	1.73	0.69
1:B:806:MET:SD	1:B:924:GLU:HB3	2.32	0.69
1:B:196:ASN:ND2	1:B:198:ALA:H	1.89	0.69
1:A:236:ASP:OD2	1:A:239:GLN:HG2	1.93	0.69
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.28	0.68
1:A:689:LEU:HD13	1:A:995:MET:HE2	1.75	0.68
1:B:538:LEU:H	1:B:732:ASN:HD21	1.41	0.68
1:B:77:LEU:HD21	1:B:271:VAL:HG21	1.75	0.68
1:B:356:VAL:HG11	1:B:377:VAL:CG2	2.23	0.68
1:B:782:ARG:HH21	1:B:964:ASP:CA	2.02	0.68
1:B:654:ILE:HD13	1:B:712:LEU:HD13	1.77	0.67
1:A:600:LEU:HD21	1:A:649:MET:HG3	1.75	0.67
1:B:506:PRO:HG2	1:B:509:VAL:HG23	1.76	0.67
1:A:123:LYS:HD2	1:A:125:ASN:HD21	1.57	0.67
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.24	0.67
1:A:174:PHE:O	1:A:238:ARG:HD3	1.95	0.66
1:B:359:LEU:HD13	1:B:360:VAL:N	2.10	0.66
1:B:871:GLU:O	1:B:875:GLU:HG2	1.96	0.66
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.44	0.66
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.78	0.66
1:A:771:LEU:HD21	1:A:954:VAL:HG23	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLU:HB2	1:B:79:SER:HB3	1.77	0.65
1:B:810:LEU:HG	1:B:928:LEU:HD21	1.78	0.65
1:B:494:GLU:CD	1:B:494:GLU:H	2.03	0.65
1:A:677:GLN:H	1:A:680:GLN:NE2	1.95	0.65
1:B:208:THR:HG23	1:B:477:ARG:NH2	1.99	0.65
1:B:679:HIS:HD2	1:B:851:GLN:OE1	1.79	0.65
1:A:294:GLN:H	1:A:297:HIS:HD2	1.44	0.65
1:B:550:LEU:HD11	1:B:558:LYS:HG2	1.77	0.64
1:A:736:GLN:H	1:A:736:GLN:CD	2.04	0.64
1:A:179:LYS:HD2	1:A:237:VAL:HB	1.80	0.64
1:A:326:TYR:HA	1:A:329:ASN:ND2	2.13	0.64
1:A:356:VAL:HG11	1:A:377:VAL:HG22	1.79	0.64
1:A:622:ASN:HD22	1:A:622:ASN:H	1.44	0.64
1:B:783:ASN:ND2	1:B:786:HIS:H	1.95	0.64
1:B:711:ARG:HH21	1:B:711:ARG:HG3	1.64	0.63
1:A:362:GLY:HA3	2:C:3:GLN:HB2	1.80	0.63
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.81	0.62
1:A:874:ILE:HA	1:A:877:MET:HE3	1.81	0.62
1:B:677:GLN:H	1:B:680:GLN:HE21	1.47	0.62
1:B:950:ARG:HD2	4:B:2190:HOH:O	1.99	0.62
1:B:196:ASN:C	1:B:196:ASN:HD22	2.08	0.62
1:A:306:PRO:HG2	1:A:483:LYS:HD3	1.82	0.62
1:A:676:GLU:OE2	1:A:676:GLU:HA	2.00	0.62
1:B:492:THR:HG22	1:B:499:GLN:OE1	2.00	0.62
1:A:194:VAL:HG12	1:A:195:MET:CE	2.29	0.61
1:B:815:ILE:HG22	1:B:870:MET:HE2	1.81	0.61
1:B:125:ASN:HD22	1:B:125:ASN:H	1.46	0.61
1:A:309:ASP:H	1:A:672:ASN:ND2	1.97	0.61
1:A:677:GLN:H	1:A:680:GLN:HE21	1.47	0.61
1:A:129:GLN:O	1:A:133:GLU:HG3	2.00	0.61
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.83	0.61
1:B:363:GLN:CD	1:B:371:MET:HE1	2.26	0.61
1:B:97:LEU:HB2	1:B:144:GLY:O	2.01	0.61
1:B:696:THR:OG1	1:B:699:GLU:HG3	2.01	0.61
1:A:141:PHE:CD2	2:C:23:VAL:HG11	2.36	0.61
1:A:817:GLU:HG3	1:A:818:PRO:CD	2.31	0.60
1:A:1006:PRO:HB3	1:B:1002:LEU:C	2.26	0.60
1:A:477:ARG:HB3	1:A:477:ARG:NH1	2.16	0.60
1:B:313:LEU:HB3	1:B:377:VAL:HG12	1.82	0.60
1:B:799:MET:CE	1:B:1008:VAL:HA	2.31	0.60
1:A:781:GLN:HE21	1:A:782:ARG:H	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:783:ASN:HD22	1:B:785:VAL:H	1.49	0.60
1:B:196:ASN:HD22	1:B:198:ALA:H	1.48	0.59
1:B:643:LYS:HE2	1:B:647:GLU:OE2	2.02	0.59
1:A:477:ARG:HH11	1:A:477:ARG:CB	2.16	0.59
1:B:204:LEU:O	1:B:208:THR:HB	2.02	0.59
1:B:380:THR:HG22	1:B:382:GLU:H	1.67	0.59
1:B:781:GLN:HE21	1:B:782:ARG:H	1.50	0.59
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.16	0.59
1:A:950:ARG:HD2	4:A:2258:HOH:O	2.03	0.59
1:A:340:HIS:ND1	1:A:341:GLU:O	2.27	0.59
1:B:510:ILE:O	1:B:514:GLN:HG3	2.03	0.59
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.38	0.58
1:A:196:ASN:HD21	1:A:198:ALA:HB3	1.68	0.58
1:B:711:ARG:HG3	1:B:711:ARG:NH2	2.19	0.58
1:A:44:ASN:C	1:A:44:ASN:HD22	2.11	0.58
1:B:259:LEU:HD12	1:B:260:GLY:N	2.19	0.58
1:A:407:GLN:HG2	1:A:409:TRP:HE1	1.69	0.58
1:A:616:LEU:HD22	1:A:641:LEU:HD23	1.86	0.58
1:B:67:LEU:CD1	1:B:75:VAL:HB	2.34	0.57
1:A:86:SER:HB3	1:A:158:LEU:HG	1.86	0.57
1:B:116:LEU:HD23	1:B:178:CYS:CB	2.23	0.57
1:B:501:LYS:HE3	1:B:503:GLU:OE1	2.04	0.57
1:B:118:THR:C	1:B:173:LEU:HD13	2.29	0.57
1:B:380:THR:HG22	1:B:382:GLU:N	2.20	0.57
1:A:957:HIS:HD2	4:A:2261:HOH:O	1.87	0.57
1:B:102:ASN:H	1:B:102:ASN:ND2	2.01	0.57
1:B:119:LYS:HB2	1:B:171:CYS:SG	2.45	0.57
1:B:799:MET:HE1	4:B:2213:HOH:O	2.04	0.57
1:B:964:ASP:O	1:B:965:SER:C	2.48	0.57
1:A:88:ALA:HB3	1:A:151:PHE:CE2	2.41	0.56
1:A:392:LEU:O	1:A:396:GLN:HG3	2.05	0.56
1:B:920:ARG:HG2	1:B:924:GLU:HG3	1.86	0.56
1:A:501:LYS:HE3	1:A:503:GLU:OE1	2.05	0.56
1:A:224:TYR:O	1:A:229:ARG:HB2	2.06	0.56
1:A:326:TYR:HA	1:A:329:ASN:HD21	1.71	0.56
1:A:359:LEU:C	1:A:359:LEU:HD23	2.31	0.56
1:A:968:VAL:HG12	1:A:989:PRO:HG3	1.86	0.56
1:A:44:ASN:ND2	1:A:46:ALA:H	2.04	0.55
1:B:783:ASN:ND2	1:B:785:VAL:H	2.04	0.55
1:B:886:ILE:HG23	1:B:928:LEU:HD13	1.88	0.55
1:A:135:ALA:HA	1:A:892:ARG:NH2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:O	1:A:230:PRO:HG2	2.05	0.55
1:A:359:LEU:HD23	1:A:360:VAL:N	2.22	0.55
1:A:359:LEU:O	2:C:1:HIS:N	2.40	0.55
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.88	0.55
1:B:604:LEU:CD2	1:B:648:LYS:HD2	2.37	0.55
1:B:969:VAL:HG21	1:B:989:PRO:CD	2.37	0.54
1:B:654:ILE:CD1	1:B:712:LEU:HD13	2.36	0.54
1:B:854:LYS:HB2	1:B:859:LEU:CD1	2.38	0.54
1:A:67:LEU:HD12	1:A:67:LEU:C	2.33	0.54
1:A:622:ASN:H	1:A:622:ASN:ND2	2.06	0.54
1:A:461:PRO:O	1:A:465:GLU:HG2	2.08	0.54
1:A:778:VAL:HG11	1:A:968:VAL:HG13	1.90	0.54
1:B:980:LEU:HD12	1:B:980:LEU:N	2.23	0.54
1:B:285:LEU:HD22	1:B:286:PRO:HD2	1.90	0.54
1:B:599:LEU:HD12	1:B:662:ILE:HD12	1.89	0.54
1:B:791:ILE:HD11	1:B:793:ILE:HD11	1.89	0.54
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.23	0.54
1:B:102:ASN:HD22	1:B:102:ASN:N	1.94	0.54
1:A:97:LEU:HB2	1:A:144:GLY:O	2.07	0.54
1:A:654:ILE:HD13	1:A:712:LEU:HD13	1.88	0.53
1:B:151:PHE:CD1	1:B:151:PHE:C	2.87	0.53
1:B:67:LEU:HD12	1:B:75:VAL:HB	1.90	0.53
1:B:141:PHE:HB2	2:D:23:VAL:HG13	1.90	0.53
1:B:722:ARG:HH11	1:B:722:ARG:HG2	1.74	0.53
1:B:538:LEU:N	1:B:732:ASN:HD21	2.06	0.53
1:B:538:LEU:H	1:B:538:LEU:HD22	1.73	0.53
1:B:847:ARG:NH1	4:B:2291:HOH:O	2.41	0.53
1:A:776:TRP:CE3	1:A:989:PRO:HB3	2.43	0.53
1:A:460:ARG:NH1	1:A:463:LEU:HG	2.24	0.53
1:B:301:LEU:HD13	1:B:478:VAL:CG2	2.38	0.53
1:B:629:LEU:HD22	1:B:630:SER:N	2.24	0.53
1:A:285:LEU:HD23	1:A:286:PRO:HD2	1.91	0.52
1:A:298:LEU:HD13	1:A:475:ASN:HA	1.92	0.52
1:B:767:ARG:NH1	1:B:1006:PRO:HA	2.24	0.52
1:B:854:LYS:HB2	1:B:859:LEU:HD11	1.91	0.52
1:A:607:TYR:CE2	1:A:644:LYS:HG2	2.45	0.52
1:B:597:LEU:HG	1:B:620:LEU:HG	1.91	0.52
1:B:506:PRO:HG2	1:B:509:VAL:CG2	2.40	0.52
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.91	0.52
1:B:713:LYS:HE2	4:B:2176:HOH:O	2.09	0.52
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:820:PHE:CE1	1:B:824:ARG:HD3	2.45	0.51
1:A:294:GLN:H	1:A:297:HIS:CD2	2.27	0.51
1:A:856:PRO:HB2	1:A:957:HIS:CD2	2.45	0.51
1:A:529:GLU:O	1:A:637:LYS:HE3	2.10	0.51
1:A:883:GLN:NE2	4:A:2042:HOH:O	2.43	0.51
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.92	0.51
1:B:392:LEU:O	1:B:396:GLN:HG3	2.09	0.51
1:B:622:ASN:HD22	1:B:622:ASN:H	1.57	0.51
1:B:877:MET:O	1:B:933:LYS:NZ	2.41	0.51
1:B:311:ARG:NH1	1:B:379:LEU:O	2.42	0.51
1:A:673:PHE:CD1	1:A:697:LYS:HE3	2.44	0.51
1:B:915:GLN:O	1:B:1011:HIS:HB2	2.09	0.51
1:A:783:ASN:ND2	1:A:785:VAL:H	2.09	0.51
1:B:294:GLN:H	1:B:297:HIS:HD2	1.59	0.51
1:B:349:GLU:OE2	1:B:349:GLU:HA	2.11	0.51
1:B:940:TYR:CE1	1:B:945:ALA:HB2	2.46	0.50
1:A:309:ASP:O	1:A:668:ARG:HG2	2.11	0.50
1:A:343:PRO:HD3	1:A:606:GLU:HG2	1.94	0.50
1:A:449:VAL:HG13	1:A:450:LEU:HD13	1.93	0.50
1:A:771:LEU:CD2	1:A:954:VAL:HG23	2.40	0.50
1:A:677:GLN:N	1:A:680:GLN:HE21	2.10	0.50
1:A:709:LEU:HG	1:A:713:LYS:HE3	1.92	0.50
1:A:805:ASN:HD22	1:A:844:GLN:NE2	2.08	0.50
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.94	0.49
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.48	0.49
1:B:805:ASN:ND2	1:B:844:GLN:NE2	2.58	0.49
1:B:622:ASN:H	1:B:622:ASN:ND2	2.10	0.49
1:B:964:ASP:O	1:B:965:SER:O	2.31	0.49
1:B:460:ARG:NH1	1:B:462:ASP:OD2	2.45	0.49
1:B:760:PRO:HA	1:B:763:LEU:HD23	1.94	0.49
1:B:874:ILE:HG22	1:B:937:ILE:HD11	1.93	0.49
1:B:451:THR:HB	1:B:455:LEU:HD12	1.94	0.49
1:B:580:SER:HB2	1:B:723:LEU:HD23	1.95	0.49
1:B:817:GLU:CB	1:B:818:PRO:HD3	2.42	0.49
1:A:460:ARG:HG3	1:A:463:LEU:HD12	1.95	0.49
1:A:931:LEU:HD12	1:A:931:LEU:N	2.28	0.49
1:A:195:MET:HB2	1:A:786:HIS:CE1	2.48	0.49
1:B:599:LEU:HD12	1:B:662:ILE:CD1	2.43	0.49
1:B:776:TRP:CE3	1:B:989:PRO:HB3	2.47	0.49
1:B:80:ASP:O	1:B:83:THR:HG22	2.13	0.49
1:A:988:GLN:NE2	1:A:989:PRO:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:GLN:NE2	1:B:371:MET:HE1	2.27	0.48
1:A:112:HIS:HA	2:C:26:LEU:CD1	2.43	0.48
1:B:226:LEU:O	1:B:237:VAL:HG21	2.12	0.48
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.95	0.48
1:A:473:PRO:O	1:A:476:VAL:HG12	2.14	0.48
1:B:829:LEU:O	1:B:852:SER:HB2	2.14	0.48
1:A:804:GLU:HG3	4:A:2268:HOH:O	2.13	0.48
1:A:44:ASN:HD22	1:A:46:ALA:H	1.62	0.48
1:A:125:ASN:HD22	1:A:125:ASN:N	2.02	0.48
1:B:793:ILE:O	1:B:847:ARG:HA	2.13	0.48
1:A:827:GLU:OE1	1:A:862:ARG:CD	2.57	0.48
1:B:380:THR:HG22	1:B:383:GLY:H	1.79	0.48
1:A:846:LEU:CD2	1:A:847:ARG:N	2.78	0.47
1:A:205:GLU:HB2	3:A:2000:DIO:H1'2	1.96	0.47
1:B:86:SER:HB3	1:B:158:LEU:HG	1.96	0.47
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.49	0.47
1:B:980:LEU:HD12	1:B:980:LEU:H	1.79	0.47
1:A:350:LEU:HB3	1:A:356:VAL:HB	1.95	0.47
1:B:359:LEU:O	2:D:1:HIS:N	2.48	0.47
1:A:824:ARG:O	1:A:828:GLN:HA	2.14	0.47
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.47	0.47
1:A:407:GLN:HG2	1:A:409:TRP:NE1	2.29	0.47
1:A:449:VAL:HG13	1:A:450:LEU:CD1	2.45	0.47
1:A:648:LYS:NZ	4:A:2233:HOH:O	2.48	0.47
1:B:196:ASN:HD22	1:B:198:ALA:N	2.09	0.47
1:A:205:GLU:HA	1:A:208:THR:HG22	1.96	0.47
1:A:223:LYS:HE3	1:A:227:GLU:OE1	2.14	0.47
1:A:342:GLY:HA2	1:A:606:GLU:CG	2.45	0.47
1:B:206:LYS:HB3	1:B:216:SER:HA	1.95	0.47
1:B:374:ILE:C	1:B:374:ILE:HD12	2.39	0.47
1:B:823:LEU:CD1	1:B:823:LEU:N	2.77	0.47
1:A:488:LYS:HD2	1:A:488:LYS:N	2.29	0.47
1:A:783:ASN:HD21	1:A:786:HIS:H	1.62	0.47
1:B:252:ASN:HB3	1:B:280:ASN:OD1	2.15	0.47
1:B:543:GLU:CD	1:B:543:GLU:H	2.23	0.47
1:B:801:SER:H	1:B:805:ASN:ND2	2.13	0.47
1:B:972:PHE:CD1	1:B:972:PHE:C	2.93	0.47
1:A:44:ASN:HD22	1:A:45:PRO:N	2.13	0.47
1:A:692:GLU:HG2	1:A:693:VAL:HG23	1.96	0.46
1:B:61:LYS:N	1:B:61:LYS:HD2	2.30	0.46
1:B:817:GLU:HB3	1:B:818:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:ILE:HG22	1:A:937:ILE:HD11	1.96	0.46
1:B:475:ASN:HB3	4:B:2095:HOH:O	2.14	0.46
1:A:321:ASP:OD2	1:A:371:MET:HE3	2.14	0.46
1:A:689:LEU:CD1	1:A:995:MET:HG2	2.45	0.46
1:A:771:LEU:HD21	1:A:954:VAL:HG21	1.98	0.46
1:B:100:PRO:HG2	1:B:103:ILE:HB	1.96	0.46
1:B:800:GLN:HA	1:B:844:GLN:NE2	2.30	0.46
1:A:927:TYR:O	1:A:930:THR:OG1	2.30	0.46
1:B:103:ILE:CD1	1:B:240:GLU:HG3	2.46	0.46
1:B:683:MET:HA	1:B:792:GLU:OE2	2.16	0.46
1:A:978:ILE:C	1:A:980:LEU:H	2.24	0.46
1:B:208:THR:CG2	1:B:477:ARG:HH12	2.28	0.46
1:B:933:LYS:O	1:B:937:ILE:HG12	2.16	0.46
1:A:205:GLU:O	1:A:208:THR:HG22	2.15	0.46
1:A:908:TRP:CZ2	1:A:912:ILE:HD11	2.51	0.46
1:A:90:LEU:HD23	1:A:91:ASP:N	2.31	0.46
1:A:306:PRO:HB3	1:A:481:VAL:CG1	2.46	0.46
1:A:342:GLY:CA	1:A:606:GLU:HG3	2.46	0.46
1:A:534:ASN:OD1	1:A:536:GLU:HG2	2.15	0.46
1:A:510:ILE:O	1:A:514:GLN:HG3	2.16	0.46
1:B:380:THR:CG2	1:B:381:GLU:N	2.79	0.46
1:B:542:LYS:HG3	1:B:543:GLU:HG3	1.98	0.46
1:B:799:MET:HE2	1:B:1008:VAL:HA	1.98	0.45
1:A:682:ALA:HA	1:A:956:VAL:HG11	1.97	0.45
1:B:823:LEU:N	1:B:823:LEU:HD12	2.31	0.45
1:A:793:ILE:O	1:A:847:ARG:HA	2.16	0.45
1:B:356:VAL:HG12	1:B:357:ASN:N	2.30	0.45
1:B:508:GLU:OE2	1:B:508:GLU:HA	2.15	0.45
1:B:972:PHE:C	1:B:972:PHE:HD1	2.24	0.45
1:A:94:ILE:HG12	1:A:248:TYR:CD2	2.52	0.45
1:B:538:LEU:N	1:B:538:LEU:HD22	2.30	0.45
2:D:23:VAL:O	2:D:23:VAL:HG12	2.17	0.45
1:A:451:THR:HB	1:A:455:LEU:HD12	1.98	0.45
1:A:778:VAL:HG21	1:A:968:VAL:CG1	2.47	0.45
1:B:204:LEU:CD2	1:B:304:ILE:HG12	2.47	0.45
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.99	0.45
1:B:805:ASN:HD22	1:B:844:GLN:NE2	2.01	0.45
1:B:852:SER:OG	1:B:853:GLU:N	2.49	0.45
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.17	0.45
1:A:200:ARG:NH2	1:A:498:THR:HA	2.32	0.45
1:A:655:ASP:C	1:A:655:ASP:OD1	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:ASN:HB2	1:A:961:ARG:NH2	2.32	0.45
1:A:99:ASP:OD2	1:A:107:SER:HB2	2.17	0.45
1:B:99:ASP:OD2	1:B:107:SER:HB2	2.17	0.45
1:B:559:LEU:HD11	1:B:729:LEU:HD22	1.97	0.45
1:A:1006:PRO:HD3	1:B:1003:PRO:HB3	1.98	0.44
1:B:196:ASN:ND2	1:B:196:ASN:C	2.75	0.44
1:A:815:ILE:C	1:A:818:PRO:HD2	2.42	0.44
1:B:794:TYR:CE1	1:B:838:ARG:HD3	2.52	0.44
1:A:552:LYS:NZ	1:A:746:GLU:OE1	2.50	0.44
1:A:600:LEU:HD23	1:A:620:LEU:HD21	1.98	0.44
1:A:683:MET:HA	1:A:792:GLU:OE2	2.17	0.44
1:A:968:VAL:CG1	1:A:989:PRO:HG3	2.48	0.44
1:B:776:TRP:CD2	1:B:989:PRO:HB3	2.53	0.44
1:B:857:HIS:CD2	1:B:972:PHE:CZ	3.05	0.44
1:B:64:TYR:CE2	1:B:450:LEU:HD21	2.53	0.44
1:B:268:THR:O	1:B:272:VAL:HG23	2.17	0.44
1:B:538:LEU:H	1:B:538:LEU:CD2	2.30	0.44
1:A:162:LEU:HD12	1:A:270:LEU:HD13	1.99	0.44
1:B:706:ASP:O	1:B:708:THR:HG23	2.17	0.44
1:B:329:ASN:OD1	1:B:332:HIS:ND1	2.38	0.44
1:B:688:LEU:O	1:B:999:LYS:HE2	2.18	0.44
1:A:1002:LEU:C	1:B:1006:PRO:HB3	2.43	0.44
1:B:782:ARG:NH2	1:B:964:ASP:CA	2.72	0.44
1:A:530:PHE:HA	1:A:637:LYS:HD2	1.99	0.43
1:B:507:ASP:HA	1:B:510:ILE:HG23	2.00	0.43
1:A:506:PRO:HG2	1:A:509:VAL:CG2	2.47	0.43
1:A:526:THR:O	1:A:527:LYS:C	2.60	0.43
1:B:592:MET:HE3	1:B:715:PHE:CD1	2.52	0.43
1:B:769:VAL:CG1	1:B:1002:LEU:HD23	2.48	0.43
1:A:580:SER:HB2	1:A:723:LEU:HD23	2.00	0.43
1:A:820:PHE:CE1	1:A:824:ARG:HD3	2.54	0.43
1:B:722:ARG:HE	1:B:756:LYS:HB2	1.83	0.43
1:B:767:ARG:HH12	1:B:1006:PRO:HA	1.83	0.43
1:A:90:LEU:HD13	1:A:169:PHE:CD2	2.54	0.43
1:A:600:LEU:HD11	1:A:648:LYS:HG3	2.00	0.43
1:B:301:LEU:HD12	1:B:302:TYR:H	1.84	0.43
1:A:208:THR:HG23	1:A:477:ARG:HH22	1.83	0.43
1:A:796:GLN:HB3	1:A:952:HIS:HB2	2.01	0.43
1:A:63:GLU:HB2	1:A:79:SER:HB3	2.00	0.43
1:A:342:GLY:HA2	1:A:606:GLU:HG3	2.00	0.43
1:A:600:LEU:HD23	1:A:620:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:GLU:OE2	1:B:676:GLU:HA	2.19	0.43
1:B:1000:ARG:HG2	1:B:1000:ARG:HH11	1.84	0.43
1:A:90:LEU:HD23	1:A:90:LEU:C	2.44	0.43
1:A:597:LEU:HG	1:A:620:LEU:HG	2.01	0.43
1:B:125:ASN:HD22	1:B:125:ASN:N	2.10	0.43
1:B:701:LYS:NZ	4:B:2260:HOH:O	2.51	0.43
1:A:180:ASP:O	1:A:183:VAL:HG12	2.19	0.43
1:A:313:LEU:HB2	1:A:379:LEU:HD11	2.00	0.43
1:A:931:LEU:N	1:A:931:LEU:CD1	2.82	0.43
1:B:71:ASN:HB2	1:B:251:SER:OG	2.18	0.43
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.49	0.43
1:A:153:VAL:HG22	1:A:154:SER:N	2.34	0.43
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.54	0.43
1:A:722:ARG:NH1	1:A:756:LYS:HE3	2.34	0.43
1:B:473:PRO:O	1:B:476:VAL:HG12	2.18	0.43
1:B:928:LEU:HD22	1:B:928:LEU:O	2.19	0.43
1:A:356:VAL:HG12	1:A:357:ASN:N	2.33	0.42
1:A:455:LEU:HA	4:A:2149:HOH:O	2.18	0.42
1:A:586:ASP:OD1	1:A:589:HIS:CD2	2.72	0.42
1:B:359:LEU:HD13	1:B:359:LEU:C	2.44	0.42
1:B:648:LYS:O	1:B:652:PHE:HB2	2.19	0.42
1:B:702:GLU:OE1	1:B:702:GLU:HA	2.19	0.42
1:B:931:LEU:N	1:B:931:LEU:HD12	2.34	0.42
1:A:572:ALA:HB3	1:A:638:GLN:OE1	2.19	0.42
1:B:820:PHE:CZ	1:B:824:ARG:HD3	2.54	0.42
1:B:821:ASN:O	1:B:825:THR:HB	2.19	0.42
1:A:377:VAL:HG13	1:A:378:ASP:O	2.19	0.42
1:B:301:LEU:HD12	1:B:302:TYR:N	2.34	0.42
1:B:877:MET:HG2	1:B:881:ALA:HB3	2.00	0.42
1:A:860:GLU:OE2	1:A:957:HIS:HE1	2.01	0.42
4:A:2390:HOH:O	2:C:26:LEU:HD11	2.19	0.42
1:B:251:SER:OG	1:B:280:ASN:HB2	2.19	0.42
1:A:80:ASP:O	1:A:83:THR:HG22	2.19	0.42
1:A:151:PHE:CD1	1:A:151:PHE:C	2.97	0.42
1:B:269:ASN:O	1:B:273:LYS:HG2	2.20	0.42
1:B:309:ASP:O	1:B:668:ARG:HG2	2.20	0.42
1:A:94:ILE:CD1	1:A:253:LEU:HD13	2.50	0.42
1:A:543:GLU:H	1:A:543:GLU:HG3	1.34	0.42
1:A:1003:PRO:HB3	1:B:1006:PRO:HD3	2.02	0.42
1:A:204:LEU:CD2	1:A:304:ILE:HG12	2.50	0.42
1:A:946:VAL:HA	1:A:951:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:ALA:HB3	1:A:963:MET:HE3	2.02	0.42
1:B:119:LYS:HD2	1:B:173:LEU:HD12	2.02	0.42
1:B:350:LEU:HD12	1:B:350:LEU:HA	1.89	0.42
1:B:801:SER:O	1:B:802:THR:C	2.63	0.42
1:A:204:LEU:HD23	3:A:2000:DIO:H2'2	2.01	0.42
2:D:22:PHE:HD2	2:D:22:PHE:HA	1.72	0.42
1:A:285:LEU:HD23	1:A:286:PRO:CD	2.50	0.42
1:B:44:ASN:HA	1:B:45:PRO:HD3	1.86	0.42
1:B:291:HIS:HA	1:B:292:PRO:HD3	1.94	0.42
1:B:380:THR:HG23	4:B:2116:HOH:O	2.19	0.42
1:B:400:LYS:HD3	4:B:2124:HOH:O	2.20	0.42
1:B:607:TYR:CE2	1:B:644:LYS:HG2	2.54	0.42
1:B:309:ASP:N	1:B:672:ASN:HD21	1.99	0.42
1:B:858:TYR:CZ	1:B:862:ARG:HD3	2.54	0.42
1:A:208:THR:HG23	1:A:477:ARG:NH2	2.35	0.41
1:B:114:LEU:HD12	1:B:149:TYR:CZ	2.54	0.41
1:B:792:GLU:HA	1:B:848:PHE:O	2.20	0.41
2:C:26:LEU:O	2:C:26:LEU:HG	2.17	0.41
1:A:736:GLN:CD	1:A:736:GLN:N	2.75	0.41
1:B:768:GLU:HB3	1:B:843:ILE:HG13	2.02	0.41
1:B:769:VAL:HG11	1:B:1002:LEU:HD23	2.01	0.41
1:A:684:TYR:CZ	1:A:688:LEU:HD11	2.55	0.41
1:B:117:GLY:O	1:B:173:LEU:HB2	2.19	0.41
1:B:930:THR:O	1:B:930:THR:HG22	2.20	0.41
1:A:162:LEU:HD12	1:A:270:LEU:CD1	2.51	0.41
1:A:205:GLU:HG3	1:A:293:PHE:HZ	1.85	0.41
1:A:810:LEU:HG	1:A:928:LEU:HD11	2.02	0.41
1:B:139:ASN:HB3	1:B:150:TYR:CZ	2.55	0.41
1:B:179:LYS:HE2	4:B:2051:HOH:O	2.21	0.41
1:B:187:ASP:OD1	1:B:222:ASN:HB2	2.21	0.41
1:B:689:LEU:CD1	1:B:995:MET:HG2	2.51	0.41
1:A:100:PRO:HA	1:A:101:PRO:HD3	1.94	0.41
1:A:402:ARG:HG2	1:A:468:LEU:HD13	2.02	0.41
1:B:604:LEU:HD21	1:B:648:LYS:HD2	2.03	0.41
1:A:588:LEU:O	1:A:592:MET:HG3	2.20	0.41
1:A:764:VAL:CA	1:B:1000:ARG:HH22	2.19	0.41
1:B:799:MET:SD	1:B:1006:PRO:HG2	2.60	0.41
1:B:810:LEU:O	1:B:814:ILE:HG13	2.20	0.41
1:A:283:VAL:HA	1:A:284:PRO:HD3	1.95	0.41
1:B:374:ILE:HD12	1:B:374:ILE:O	2.20	0.41
1:B:862:ARG:HA	1:B:862:ARG:NE	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLY:HA3	1:A:363:GLN:OE1	2.21	0.41
1:B:422:PHE:CZ	1:B:451:THR:HG22	2.56	0.41
1:B:729:LEU:HD23	1:B:738:ALA:HA	2.02	0.41
1:A:108:HIS:HE1	1:A:189:GLU:OE2	2.04	0.41
1:A:402:ARG:CG	1:A:468:LEU:HD13	2.51	0.41
1:A:449:VAL:CG1	1:A:450:LEU:HD13	2.51	0.41
1:A:688:LEU:HD13	1:A:696:THR:HG22	2.03	0.41
1:A:783:ASN:HD22	1:A:785:VAL:H	1.68	0.41
1:A:978:ILE:C	1:A:980:LEU:N	2.78	0.41
1:B:153:VAL:HG22	1:B:154:SER:N	2.35	0.41
1:B:164:ARG:HG3	1:B:164:ARG:HH11	1.84	0.41
1:B:550:LEU:CD1	1:B:558:LYS:HG2	2.47	0.41
1:B:806:MET:HE1	1:B:809:GLU:OE1	2.21	0.41
1:B:806:MET:HE1	1:B:893:ARG:NH1	2.36	0.41
1:B:810:LEU:HA	1:B:889:LEU:HD12	2.02	0.41
1:A:90:LEU:HD13	1:A:169:PHE:CE2	2.56	0.41
1:A:729:LEU:HD12	1:A:738:ALA:HB1	2.03	0.41
4:A:2045:HOH:O	2:C:1:HIS:HB2	2.20	0.41
1:B:201:LEU:HD12	1:B:201:LEU:HA	1.91	0.41
1:B:99:ASP:OD2	1:B:107:SER:CB	2.69	0.40
1:B:600:LEU:CD2	1:B:649:MET:HG3	2.52	0.40
1:B:711:ARG:HH21	1:B:711:ARG:CG	2.32	0.40
1:A:846:LEU:HD23	1:A:847:ARG:H	1.86	0.40
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.56	0.40
1:B:679:HIS:CD2	1:B:851:GLN:OE1	2.68	0.40
1:B:814:ILE:HG23	1:B:877:MET:HE1	2.03	0.40
1:B:696:THR:O	1:B:700:LEU:HD22	2.22	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	966/990 (98%)	918 (95%)	45 (5%)	3 (0%)	36	55
1	B	962/990 (97%)	923 (96%)	38 (4%)	1 (0%)	48	68
2	C	7/29 (24%)	7 (100%)	0	0	100	100
2	D	5/29 (17%)	4 (80%)	0	1 (20%)	0	0
All	All	1940/2038 (95%)	1852 (96%)	83 (4%)	5 (0%)	36	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	965	SER
1	A	1015	MET
1	A	979	ASN
1	A	228	THR
2	D	23	VAL

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	857/883 (97%)	797 (93%)	60 (7%)	14	29
1	B	855/883 (97%)	794 (93%)	61 (7%)	13	29
2	C	10/27 (37%)	7 (70%)	3 (30%)	0	0
2	D	9/27 (33%)	5 (56%)	4 (44%)	0	0
All	All	1731/1820 (95%)	1603 (93%)	128 (7%)	13	27

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ILE
1	A	97	LEU
1	A	123	LYS
1	A	125	ASN
1	A	158	LEU
1	A	162	LEU

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Mol	Chain	Res	Type
1	A	201	LEU
1	A	226	LEU
1	A	229	ARG
1	A	238	ARG
1	A	242	LEU
1	A	270	LEU
1	A	285	LEU
1	A	287	GLU
1	A	337	LEU
1	A	347	LEU
1	A	350	LEU
1	A	377	VAL
1	A	399	GLN
1	A	407	GLN
1	A	417	LEU
1	A	450	LEU
1	A	466	MET
1	A	468	LEU
1	A	508	GLU
1	A	511	LYS
1	A	529	GLU
1	A	542	LYS
1	A	543	GLU
1	A	558	LYS
1	A	595	LEU
1	A	597	LEU
1	A	599	LEU
1	A	612	GLU
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	642	LEU
1	A	668	ARG
1	A	689	LEU
1	A	707	VAL
1	A	712	LEU
1	A	720	LEU
1	A	736	GLN
1	A	759	LEU
1	A	771	LEU
1	A	781	GLN
1	A	788	ASN

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Mol	Chain	Res	Type
1	A	810	LEU
1	A	817	GLU
1	A	823	LEU
1	A	846	LEU
1	A	859	LEU
1	A	860	GLU
1	A	867	LEU
1	A	889	LEU
1	A	962	GLU
1	A	969	VAL
1	A	1002	LEU
1	A	1007	LEU
1	B	52	ASN
1	B	85	LYS
1	B	94	ILE
1	B	97	LEU
1	B	102	ASN
1	B	125	ASN
1	B	158	LEU
1	B	162	LEU
1	B	173	LEU
1	B	196	ASN
1	B	201	LEU
1	B	208	THR
1	B	226	LEU
1	B	242	LEU
1	B	259	LEU
1	B	347	LEU
1	B	350	LEU
1	B	359	LEU
1	B	377	VAL
1	B	378	ASP
1	B	380	THR
1	B	417	LEU
1	B	446	LEU
1	B	450	LEU
1	B	454	TYR
1	B	468	LEU
1	B	478	VAL
1	B	494	GLU
1	B	510	ILE
1	B	524	LEU

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Mol	Chain	Res	Type
1	B	543	GLU
1	B	558	LYS
1	B	595	LEU
1	B	597	LEU
1	B	599	LEU
1	B	613	LEU
1	B	616	LEU
1	B	622	ASN
1	B	629	LEU
1	B	642	LEU
1	B	668	ARG
1	B	689	LEU
1	B	700	LEU
1	B	711	ARG
1	B	712	LEU
1	B	720	LEU
1	B	722	ARG
1	B	728	LEU
1	B	771	LEU
1	B	781	GLN
1	B	783	ASN
1	B	806	MET
1	B	810	LEU
1	B	846	LEU
1	B	889	LEU
1	B	906	LYS
1	B	924	GLU
1	B	928	LEU
1	B	972	PHE
1	B	1002	LEU
1	B	1007	LEU
2	C	3	GLN
2	C	23	VAL
2	C	27	MET
2	D	3	GLN
2	D	22	PHE
2	D	23	VAL
2	D	27	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	44	ASN
1	A	93	HIS
1	A	111	GLN
1	A	125	ASN
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	336	HIS
1	A	376	ASN
1	A	386	HIS
1	A	399	GLN
1	A	407	GLN
1	A	475	ASN
1	A	502	GLN
1	A	514	GLN
1	A	575	ASN
1	A	589	HIS
1	A	621	GLN
1	A	622	ASN
1	A	672	ASN
1	A	680	GLN
1	A	718	GLN
1	A	730	HIS
1	A	743	GLN
1	A	752	HIS
1	A	770	GLN
1	A	781	GLN
1	A	783	ASN
1	A	788	ASN
1	A	805	ASN
1	A	828	GLN
1	A	883	GLN
1	A	922	ASN
1	A	957	HIS
1	A	988	GLN
1	B	53	HIS
1	B	93	HIS
1	B	102	ASN
1	B	125	ASN

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Mol	Chain	Res	Type
1	B	184	ASN
1	B	196	ASN
1	B	232	GLN
1	B	282	ASN
1	B	294	GLN
1	B	297	HIS
1	B	300	GLN
1	B	376	ASN
1	B	399	GLN
1	B	475	ASN
1	B	502	GLN
1	B	591	ASN
1	B	605	ASN
1	B	622	ASN
1	B	672	ASN
1	B	679	HIS
1	B	680	GLN
1	B	718	GLN
1	B	732	ASN
1	B	752	HIS
1	B	770	GLN
1	B	780	GLN
1	B	781	GLN
1	B	783	ASN
1	B	805	ASN
1	B	813	GLN
1	B	828	GLN
1	B	841	ASN
1	B	857	HIS
1	B	914	GLN
1	B	922	ASN
1	B	957	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	DIO	A	2000	-	6,6,6	0.85	0	6,6,6	0.21	0
3	DIO	B	2001	-	6,6,6	0.79	0	6,6,6	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DIO	A	2000	-	-	-	0/1/1/1
3	DIO	B	2001	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	DIO	2	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

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	970/990 (97%)	-0.21	18 (1%) 66 62	15, 29, 47, 77	0
1	B	966/990 (97%)	0.05	27 (2%) 55 50	21, 35, 54, 78	0
2	C	11/29 (37%)	2.32	8 (72%) 0 0	52, 54, 60, 61	0
2	D	9/29 (31%)	2.33	6 (66%) 0 0	51, 54, 55, 63	0
All	All	1956/2038 (95%)	-0.06	59 (3%) 52 48	15, 31, 53, 78	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1016	ALA	7.8
1	B	1012	ILE	7.4
1	A	1014	PHE	7.3
1	B	964	ASP	6.9
1	B	1014	PHE	6.2
1	A	976	ASN	6.1
1	A	978	ILE	6.0
1	B	965	SER	5.2
2	C	4	GLY	5.2
1	A	979	ASN	5.2
1	B	978	ILE	5.1
1	A	977	ASP	4.7
1	A	1015	MET	4.7
1	B	979	ASN	4.3
1	B	971	GLU	4.1
1	B	44	ASN	3.7
1	A	1012	ILE	3.6
1	B	972	PHE	3.6
1	B	1011	HIS	3.6
1	A	971	GLU	3.4
2	D	27	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	964	ASP	3.3
2	C	28	ASN	3.3
1	B	969	VAL	3.3
2	D	25	TRP	3.2
2	D	23	VAL	3.2
1	B	967	PRO	3.1
1	A	43	ASN	3.0
1	B	1013	ASN	2.8
2	D	22	PHE	2.8
1	B	706	ASP	2.7
1	B	968	VAL	2.7
1	B	980	LEU	2.6
2	C	24	GLN	2.6
1	B	508	GLU	2.6
2	C	26	LEU	2.6
1	A	543	GLU	2.5
1	A	763	LEU	2.5
1	B	1009	LYS	2.5
1	B	168	PHE	2.5
1	B	962	GLU	2.4
1	B	966	CYS	2.3
2	C	22	PHE	2.3
2	C	25	TRP	2.3
1	A	764	VAL	2.3
1	A	1013	ASN	2.2
2	D	26	LEU	2.2
2	C	23	VAL	2.2
1	B	877	MET	2.2
1	B	970	GLY	2.2
1	B	868	ILE	2.2
2	C	27	MET	2.1
2	D	1	HIS	2.1
1	A	342	GLY	2.1
1	A	968	VAL	2.0
1	B	947	ASP	2.0
1	A	1011	HIS	2.0
1	B	51	GLY	2.0
1	B	896	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DIO	B	2001	6/6	0.91	0.14	44,45,46,46	0
3	DIO	A	2000	6/6	0.92	0.12	46,46,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.