



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:48 PM UTC

PDB ID : 2G47 / pdb_00002g47
Title : Crystal structure of human insulin-degrading enzyme in complex with amyloid-beta (1-40)
Authors : Shen, Y.; Tang, W.-J.
Deposited on : 2006-02-21
Resolution : 2.10 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

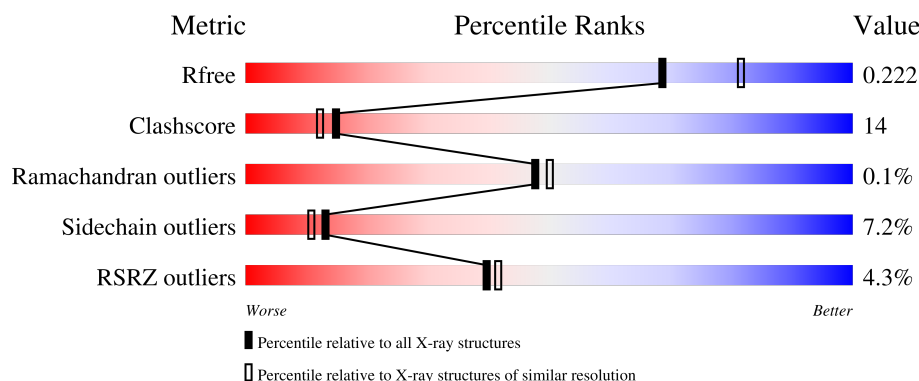
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	990	4% 69% 25% • •
1	B	990	4% 69% 25% • •
2	C	40	15% 15% 8% 5% 72%
2	D	40	5% 18% 8% • 72%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16962 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	964	Total	C	N	O	S	0	0	0
			7853	5053	1319	1447	34			
1	B	965	Total	C	N	O	S	0	0	0
			7855	5055	1319	1447	34			

There are 26 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	-	cloning artifact	UNP P14735
A	38	ALA	-	cloning artifact	UNP P14735
A	39	GLY	-	cloning artifact	UNP P14735
A	40	ILE	-	cloning artifact	UNP P14735
A	41	PRO	-	cloning artifact	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
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	-	cloning artifact	UNP P14735
B	38	ALA	-	cloning artifact	UNP P14735
B	39	GLY	-	cloning artifact	UNP P14735
B	40	ILE	-	cloning artifact	UNP P14735
B	41	PRO	-	cloning artifact	UNP P14735

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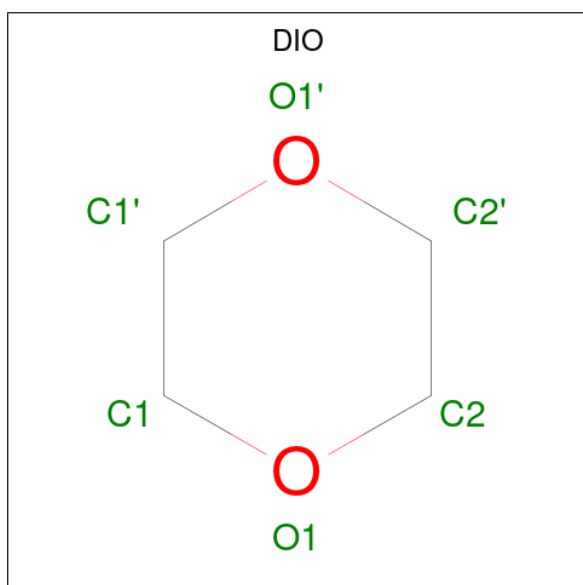
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Chain	Residue	Modelled	Actual	Comment	Reference
B	111	GLN	GLU	engineered mutation	UNP P14735

- Molecule 2 is a protein called amyloid protein beta A4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	0	0	0
			86	57	12	17			
2	D	11	Total	C	N	O	0	0	0
			90	59	12	19			

- 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	564	Total	O	0	0
			564	564		
4	B	497	Total	O	0	0
			497	497		

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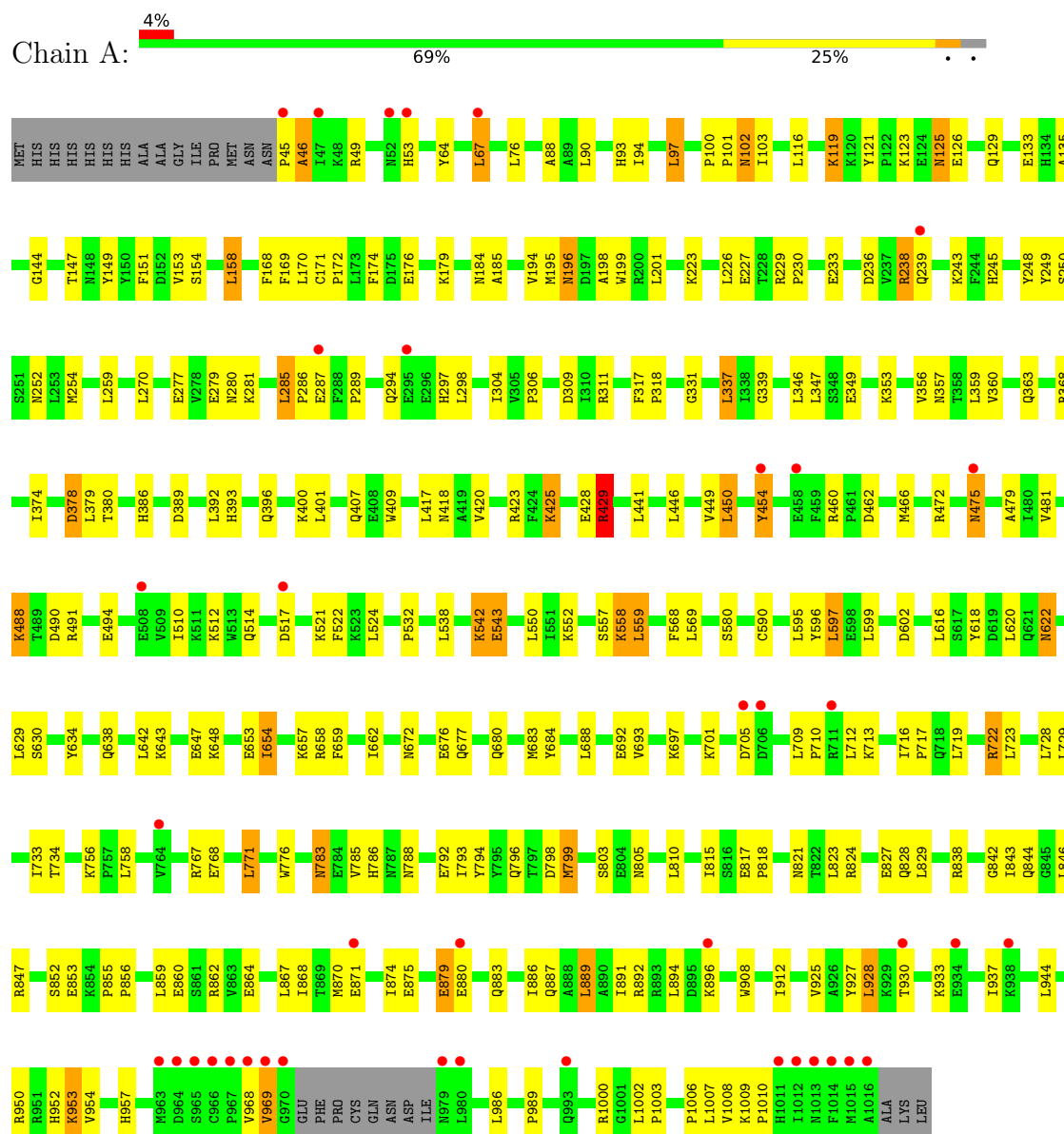
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	O	0	0
			2	2		
4	D	3	Total	O	0	0
			3	3		

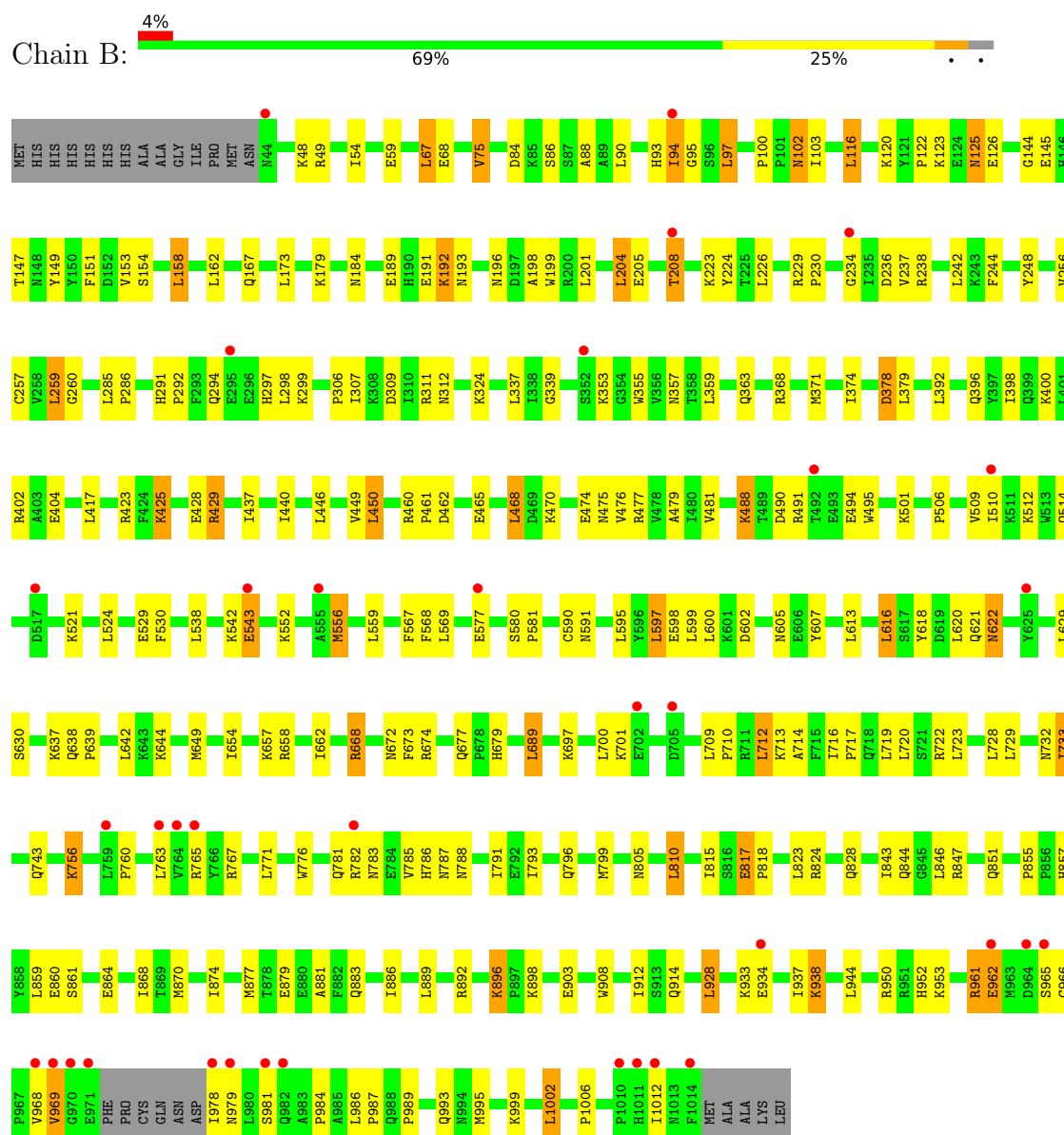
3 Residue-property plots

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.

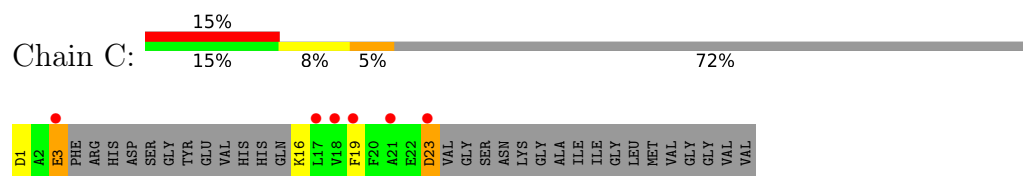
• Molecule 1: Insulin-degrading enzyme



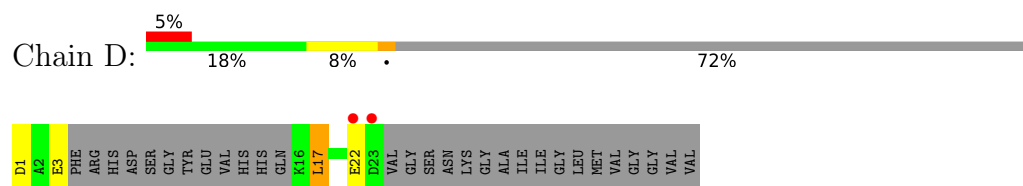
• Molecule 1: Insulin-degrading enzyme



- Molecule 2: amyloid protein beta A4



- Molecule 2: amyloid protein beta A4



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	262.43Å 262.43Å 90.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.77 – 2.10 29.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.77-2.10) 90.6 (29.77-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.223 0.202 , 0.222	Depositor DCC
R_{free} test set	19336 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16962	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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

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	0.41	0/8049	0.88	17/10887 (0.2%)
1	B	0.43	0/8051	0.91	19/10891 (0.2%)
2	C	1.21	0/86	1.33	2/113 (1.8%)
2	D	1.76	0/90	1.42	0/118
All	All	0.45	0/16276	0.90	38/22009 (0.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	494	GLU	N-CA-C	7.68	120.39	111.02
1	A	494	GLU	N-CA-C	7.65	119.62	111.28
1	A	116	LEU	N-CA-C	7.40	120.93	112.57
1	A	121	TYR	CA-C-N	6.95	126.77	119.05
1	A	121	TYR	C-N-CA	6.95	126.77	119.05
1	B	116	LEU	N-CA-C	6.95	120.34	112.97
1	A	654	ILE	N-CA-C	6.45	117.36	109.30
1	B	944	LEU	N-CA-C	6.38	121.59	113.55
2	C	19	PHE	N-CA-C	6.20	120.03	110.42
1	A	953	LYS	N-CA-C	6.12	118.87	108.90
1	A	378	ASP	N-CA-C	-6.11	101.74	110.59
1	B	569	LEU	N-CA-C	-6.08	100.80	110.10
1	A	429	ARG	N-CA-C	-6.07	102.41	109.93
1	B	122	PRO	N-CA-C	6.02	121.78	113.65
1	B	495	TRP	N-CA-C	5.99	118.77	111.82
1	B	307	ILE	N-CA-C	-5.96	105.04	110.82
1	B	378	ASP	N-CA-C	-5.82	101.91	110.52
1	A	590	CYS	N-CA-C	-5.72	105.12	111.36
1	A	557	SER	N-CA-C	5.69	117.75	108.76
1	B	476	VAL	N-CA-C	5.64	118.03	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	THR	N-CA-C	-5.58	102.50	110.59
1	A	304	ILE	N-CA-C	5.53	116.44	108.48
1	B	605	ASN	N-CA-C	5.48	117.69	111.11
1	B	590	CYS	N-CA-C	-5.42	105.27	111.07
1	A	944	LEU	N-CA-C	5.39	120.51	113.88
1	B	568	PHE	N-CA-C	5.29	118.69	111.39
1	A	46	ALA	N-CA-C	-5.26	106.83	113.20
1	A	569	LEU	N-CA-C	-5.25	102.07	110.10
1	B	961	ARG	CA-C-N	-5.24	113.89	122.54
1	B	961	ARG	C-N-CA	-5.24	113.89	122.54
1	B	312	ASN	N-CA-C	5.21	117.10	109.24
1	B	429	ARG	N-CA-C	-5.18	103.25	109.83
1	A	853	GLU	N-CA-C	-5.16	106.49	112.89
1	B	677	GLN	CA-C-N	5.13	125.17	119.32
1	B	677	GLN	C-N-CA	5.13	125.17	119.32
2	C	23	ASP	N-CA-C	5.06	125.18	111.00
1	A	559	LEU	N-CA-C	5.06	116.76	108.52
1	B	75	VAL	N-CA-C	5.05	115.99	108.46

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	7853	0	7773	231	1
1	B	7855	0	7767	200	1
2	C	86	0	78	3	0
2	D	90	0	82	9	0
3	A	6	0	8	1	0
3	B	6	0	8	2	0
4	A	564	0	0	28	0
4	B	497	0	0	24	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
All	All	16962	0	15716	437	1

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 (437) 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:782:ARG:NH2	1:B:961:ARG:O	1.65	1.28
1:B:892:ARG:HD2	4:B:2433:HOH:O	1.50	1.12
2:D:17:LEU:HD23	2:D:17:LEU:O	1.62	0.99
1:A:194:VAL:HG12	1:A:195:MET:HE2	1.46	0.98
1:B:208:THR:HG23	1:B:477:ARG:HH22	1.28	0.96
2:D:17:LEU:HD23	2:D:17:LEU:C	1.86	0.95
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.49	0.94
1:A:102:ASN:H	1:A:102:ASN:HD22	1.14	0.94
2:D:17:LEU:H	2:D:17:LEU:HD22	1.32	0.94
1:B:864:GLU:HG2	1:B:986:LEU:HD21	1.50	0.93
1:B:674:ARG:HD3	4:B:2199:HOH:O	1.69	0.92
1:A:705:ASP:HB2	4:A:2459:HOH:O	1.68	0.92
1:A:879:GLU:HG2	4:A:2307:HOH:O	1.69	0.91
1:A:425:LYS:HE2	1:A:428:GLU:OE2	1.71	0.89
1:A:309:ASP:H	1:A:672:ASN:HD21	1.17	0.88
1:A:512:LYS:NZ	4:A:2554:HOH:O	2.07	0.88
1:A:287:GLU:HG2	1:A:289:PRO:HD3	1.55	0.88
2:D:17:LEU:HD22	2:D:17:LEU:N	1.85	0.87
1:A:864:GLU:HG2	1:A:986:LEU:HD21	1.58	0.86
1:B:782:ARG:NH2	1:B:961:ARG:C	2.33	0.86
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.55	0.86
1:B:309:ASP:H	1:B:672:ASN:HD21	1.19	0.85
1:B:815:ILE:HG22	1:B:870:MET:HE2	1.58	0.85
1:A:874:ILE:O	1:A:933:LYS:HE3	1.78	0.84
1:B:521:LYS:NZ	4:B:2136:HOH:O	2.11	0.84
1:B:102:ASN:HD22	1:B:102:ASN:H	1.24	0.83
1:B:59:GLU:OE2	4:B:2440:HOH:O	1.97	0.81
1:A:1000:ARG:HD2	4:B:2259:HOH:O	1.79	0.81
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.62	0.80
1:B:950:ARG:HD2	4:B:2213:HOH:O	1.82	0.80
1:A:771:LEU:HD21	1:A:954:VAL:HG23	1.65	0.79
1:A:599:LEU:HD23	1:A:662:ILE:HD12	1.62	0.79
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.82	0.79
1:A:174:PHE:O	1:A:238:ARG:HD3	1.84	0.78
1:A:309:ASP:H	1:A:672:ASN:ND2	1.82	0.78
1:B:309:ASP:H	1:B:672:ASN:ND2	1.83	0.77
1:B:791:ILE:HD11	1:B:793:ILE:HD11	1.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:783:ASN:ND2	1:B:786:HIS:H	1.83	0.76
1:A:558:LYS:NZ	4:A:2216:HOH:O	2.17	0.76
1:A:294:GLN:H	1:A:297:HIS:HD2	1.34	0.76
2:D:17:LEU:N	2:D:17:LEU:CD2	2.49	0.75
1:B:658:ARG:NH2	4:B:2456:HOH:O	2.18	0.75
1:B:224:TYR:CZ	1:B:229:ARG:HD2	2.22	0.75
1:B:208:THR:HG23	1:B:477:ARG:NH2	2.02	0.74
1:A:558:LYS:NZ	1:A:558:LYS:HB2	2.02	0.74
1:A:135:ALA:HA	1:A:892:ARG:NH2	2.02	0.74
1:B:294:GLN:H	1:B:297:HIS:HD2	1.33	0.74
1:B:429:ARG:HD2	4:B:2318:HOH:O	1.87	0.74
1:A:102:ASN:HD22	1:A:102:ASN:N	1.85	0.74
1:B:425:LYS:HE2	1:B:428:GLU:OE2	1.87	0.74
1:A:821:ASN:HB2	4:A:2008:HOH:O	1.89	0.73
1:A:643:LYS:NZ	4:A:2560:HOH:O	2.21	0.72
1:A:446:LEU:H	1:A:446:LEU:HD22	1.52	0.72
1:A:339:GLY:O	2:C:1:ASP:HA	1.90	0.72
1:B:886:ILE:HG23	1:B:928:LEU:HD13	1.70	0.72
1:B:591:ASN:O	1:B:595:LEU:HD23	1.90	0.71
2:D:17:LEU:C	2:D:17:LEU:CD2	2.61	0.71
1:B:299:LYS:HD2	1:B:510:ILE:HD13	1.71	0.71
1:A:491:ARG:HD2	4:A:2179:HOH:O	1.89	0.71
1:A:886:ILE:HG23	1:A:928:LEU:HD22	1.72	0.71
1:B:883:GLN:NE2	4:B:2432:HOH:O	2.23	0.71
1:B:886:ILE:HG23	1:B:928:LEU:CD1	2.20	0.71
1:B:94:ILE:HD11	1:B:244:PHE:CZ	2.26	0.70
1:B:49:ARG:NH2	1:B:446:LEU:HD23	2.07	0.70
1:A:53:HIS:H	1:A:53:HIS:CD2	2.07	0.70
1:B:760:PRO:HA	1:B:763:LEU:HD23	1.74	0.69
1:B:423:ARG:NE	4:B:2440:HOH:O	2.17	0.69
1:A:968:VAL:O	1:A:969:VAL:HG22	1.93	0.69
1:B:817:GLU:HG3	1:B:818:PRO:CD	2.21	0.69
1:B:236:ASP:OD1	4:B:2074:HOH:O	2.12	0.68
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.41	0.68
1:A:102:ASN:H	1:A:102:ASN:ND2	1.90	0.67
1:A:446:LEU:CD2	4:A:2165:HOH:O	2.42	0.67
1:A:622:ASN:HD22	1:A:622:ASN:H	1.42	0.67
1:B:125:ASN:HD22	1:B:125:ASN:H	1.42	0.67
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.43	0.67
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.43	0.66
1:B:538:LEU:H	1:B:732:ASN:HD21	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ARG:HD2	4:A:2150:HOH:O	1.94	0.66
1:A:538:LEU:HD12	1:A:538:LEU:N	2.10	0.66
1:A:337:LEU:HD23	1:A:401:LEU:HD22	1.78	0.65
1:A:783:ASN:ND2	1:A:785:VAL:H	1.95	0.65
1:B:94:ILE:HG12	1:B:95:GLY:N	2.12	0.65
1:B:102:ASN:HD22	1:B:102:ASN:N	1.90	0.65
1:A:1002:LEU:C	1:B:1006:PRO:HB3	2.22	0.65
1:B:229:ARG:HB3	1:B:230:PRO:HD3	1.78	0.64
1:A:88:ALA:HB3	1:A:151:PHE:CE2	2.32	0.64
1:A:783:ASN:ND2	1:A:786:HIS:H	1.96	0.64
1:A:799:MET:HE1	1:A:1006:PRO:HG2	1.78	0.64
1:A:184:ASN:HD21	1:A:223:LYS:NZ	1.96	0.64
1:A:815:ILE:HG22	1:A:870:MET:HE2	1.78	0.64
1:B:84:ASP:OD2	1:B:896:LYS:HG2	1.97	0.64
1:B:196:ASN:HD22	1:B:199:TRP:H	1.43	0.64
1:A:815:ILE:HA	1:A:870:MET:HE2	1.79	0.63
1:A:236:ASP:CG	1:A:239:GLN:HG2	2.23	0.63
1:A:233:GLU:OE1	4:A:2534:HOH:O	2.15	0.62
1:A:950:ARG:HD2	4:A:2278:HOH:O	1.98	0.62
1:B:192:LYS:HD3	1:B:193:ASN:OD1	1.99	0.62
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.80	0.62
1:B:874:ILE:O	1:B:933:LYS:HD2	2.00	0.62
1:B:357:ASN:HB2	1:B:378:ASP:OD1	2.00	0.61
1:A:968:VAL:C	1:A:969:VAL:CG2	2.72	0.61
1:B:102:ASN:H	1:B:102:ASN:ND2	1.98	0.61
1:A:407:GLN:HG3	1:A:409:TRP:CD1	2.35	0.61
1:B:622:ASN:HD22	1:B:622:ASN:H	1.45	0.61
1:A:475:ASN:C	1:A:475:ASN:ND2	2.59	0.61
1:B:423:ARG:NH2	4:B:2440:HOH:O	2.27	0.61
1:B:126:GLU:HG3	4:B:2336:HOH:O	2.00	0.61
1:A:298:LEU:HD21	1:A:318:PRO:HG2	1.83	0.61
1:B:449:VAL:HG13	1:B:450:LEU:HD13	1.81	0.61
1:B:294:GLN:H	1:B:297:HIS:CD2	2.18	0.60
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.83	0.60
1:A:783:ASN:HD22	1:A:785:VAL:H	1.50	0.60
1:A:460:ARG:NH1	1:A:462:ASP:OD2	2.35	0.60
1:A:542:LYS:HB2	1:A:542:LYS:NZ	2.17	0.60
1:A:97:LEU:HB2	1:A:144:GLY:O	2.01	0.59
1:A:517:ASP:HB2	4:A:2189:HOH:O	2.02	0.59
1:B:205:GLU:O	1:B:208:THR:HG22	2.01	0.59
1:A:490:ASP:OD1	1:A:491:ARG:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:VAL:HG23	1:A:969:VAL:HG23	1.84	0.59
1:B:679:HIS:HD2	1:B:851:GLN:OE1	1.85	0.59
1:B:285:LEU:HD13	1:B:286:PRO:O	2.02	0.59
2:D:17:LEU:H	2:D:17:LEU:CD2	2.09	0.59
1:A:684:TYR:OH	1:A:697:LYS:HG2	2.03	0.58
1:B:94:ILE:HD11	1:B:244:PHE:HZ	1.68	0.58
1:B:100:PRO:HG2	1:B:103:ILE:HB	1.84	0.58
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.85	0.58
1:A:1006:PRO:HB3	1:B:1002:LEU:C	2.28	0.58
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.51	0.58
1:A:168:PHE:O	1:A:172:PRO:HG3	2.04	0.58
1:A:889:LEU:HB3	1:A:928:LEU:HD11	1.84	0.58
1:B:999:LYS:NZ	4:B:2415:HOH:O	2.36	0.58
1:A:176:GLU:OE2	1:A:238:ARG:HG3	2.03	0.57
1:A:331:GLY:HA3	1:A:363:GLN:OE1	2.04	0.57
1:A:100:PRO:HG2	1:A:103:ILE:HB	1.85	0.57
1:A:558:LYS:HB2	1:A:558:LYS:HZ2	1.68	0.57
1:B:259:LEU:HD12	1:B:259:LEU:C	2.29	0.57
1:B:479:ALA:HB2	3:B:2001:DIO:H12	1.85	0.57
1:B:49:ARG:HH22	1:B:446:LEU:HD23	1.67	0.57
1:B:709:LEU:N	1:B:710:PRO:HD2	2.20	0.57
1:A:883:GLN:NE2	4:A:2042:HOH:O	2.38	0.56
1:B:196:ASN:HD21	1:B:198:ALA:HB3	1.70	0.56
1:A:125:ASN:H	1:A:125:ASN:HD22	1.52	0.56
1:B:299:LYS:HD2	1:B:510:ILE:CD1	2.34	0.56
1:A:658:ARG:NH2	4:A:2147:HOH:O	2.39	0.56
1:B:402:ARG:HG2	1:B:468:LEU:HD13	1.88	0.56
1:B:898:LYS:HE3	4:B:2040:HOH:O	2.06	0.56
1:B:474:GLU:C	1:B:475:ASN:HD22	2.14	0.56
1:A:223:LYS:HE2	4:A:2387:HOH:O	2.05	0.56
1:A:349:GLU:CD	1:A:521:LYS:HD3	2.31	0.56
1:A:429:ARG:HB3	1:A:429:ARG:HH11	1.71	0.56
1:B:602:ASP:OD1	1:B:658:ARG:HD3	2.06	0.56
1:A:597:LEU:HG	1:A:620:LEU:HG	1.88	0.55
1:B:868:ILE:HD12	1:B:984:PRO:HD3	1.87	0.55
1:A:429:ARG:NH1	4:A:2033:HOH:O	2.38	0.55
1:A:441:LEU:CD2	1:A:449:VAL:HG11	2.31	0.55
1:A:908:TRP:CZ2	1:A:912:ILE:HD11	2.42	0.55
1:B:49:ARG:NH2	4:B:2269:HOH:O	2.18	0.55
1:A:722:ARG:HB3	1:A:758:LEU:HD13	1.87	0.55
1:A:767:ARG:NH1	1:A:1006:PRO:HA	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:GLY:O	2:D:1:ASP:HA	2.07	0.55
1:A:874:ILE:HG22	1:A:937:ILE:HD11	1.88	0.54
1:A:927:TYR:O	1:A:930:THR:HB	2.06	0.54
1:B:673:PHE:CD1	1:B:697:LYS:HE3	2.42	0.54
1:A:446:LEU:HD22	4:A:2165:HOH:O	2.03	0.54
1:B:654:ILE:HD13	1:B:712:LEU:HD13	1.89	0.54
1:A:580:SER:HB2	1:A:723:LEU:HD23	1.90	0.54
1:A:950:ARG:NH1	4:A:2289:HOH:O	2.41	0.54
1:B:961:ARG:O	1:B:961:ARG:HG2	2.06	0.54
1:A:538:LEU:N	1:A:538:LEU:CD1	2.71	0.54
1:A:243:LYS:HB2	1:A:243:LYS:NZ	2.22	0.54
1:A:692:GLU:HG2	1:A:693:VAL:HG23	1.90	0.54
1:A:803:SER:HA	1:A:927:TYR:CE2	2.43	0.54
1:A:407:GLN:HG3	1:A:409:TRP:NE1	2.23	0.54
1:A:475:ASN:C	1:A:475:ASN:HD22	2.16	0.54
1:B:191:GLU:OE2	4:B:2348:HOH:O	2.19	0.54
1:A:184:ASN:HD21	1:A:223:LYS:HZ1	1.54	0.53
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.35	0.53
1:A:868:ILE:O	1:A:871:GLU:HB3	2.08	0.53
1:B:461:PRO:O	1:B:465:GLU:HG3	2.08	0.53
4:B:2406:HOH:O	2:D:1:ASP:HB2	2.07	0.53
1:A:185:ALA:HB2	1:A:828:GLN:HE22	1.74	0.53
1:B:622:ASN:H	1:B:622:ASN:ND2	2.07	0.53
1:A:543:GLU:CD	1:A:543:GLU:H	2.16	0.53
1:A:887:GLN:OE1	4:A:2041:HOH:O	2.19	0.53
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.25	0.53
1:A:475:ASN:ND2	1:A:475:ASN:O	2.43	0.52
1:B:368:ARG:HD3	4:B:2313:HOH:O	2.09	0.52
1:A:119:LYS:HB2	1:A:171:CYS:HB2	1.91	0.52
1:A:259:LEU:C	1:A:259:LEU:HD23	2.35	0.52
1:A:968:VAL:C	1:A:969:VAL:HG23	2.34	0.52
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.45	0.52
1:A:93:HIS:HE1	1:A:368:ARG:NH2	2.08	0.52
1:A:558:LYS:HB2	1:A:558:LYS:HZ3	1.75	0.52
1:B:359:LEU:C	1:B:359:LEU:HD23	2.35	0.52
1:B:392:LEU:O	1:B:396:GLN:HG3	2.10	0.52
1:B:879:GLU:HB2	4:B:2488:HOH:O	2.09	0.52
1:A:285:LEU:HD23	1:A:286:PRO:HD2	1.92	0.52
1:B:97:LEU:HB2	1:B:144:GLY:O	2.09	0.52
1:B:49:ARG:HG2	1:B:68:GLU:HB3	1.91	0.51
1:A:843:ILE:HG22	1:A:844:GLN:H	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:HG21	1:B:248:TYR:HB3	1.93	0.51
1:A:317:PHE:HD2	1:A:475:ASN:ND2	2.09	0.51
1:B:309:ASP:N	1:B:672:ASN:HD21	1.99	0.51
1:A:653:GLU:N	4:A:2250:HOH:O	2.27	0.51
1:A:677:GLN:HB2	1:A:680:GLN:HG3	1.92	0.51
1:B:978:ILE:O	1:B:979:ASN:CB	2.59	0.51
1:A:53:HIS:HB3	4:A:2366:HOH:O	2.10	0.51
1:B:760:PRO:HA	1:B:763:LEU:CD2	2.41	0.51
1:B:782:ARG:CZ	1:B:961:ARG:O	2.51	0.51
1:A:542:LYS:HB2	1:A:542:LYS:HZ2	1.76	0.51
1:B:616:LEU:HD21	1:B:638:GLN:HG2	1.93	0.50
1:A:676:GLU:OE2	1:A:676:GLU:HA	2.10	0.50
1:A:359:LEU:C	1:A:359:LEU:HD23	2.37	0.50
1:B:490:ASP:OD1	1:B:491:ARG:HG3	2.11	0.50
1:B:877:MET:HG3	1:B:881:ALA:HB3	1.93	0.50
1:B:238:ARG:O	1:B:242:LEU:HD23	2.12	0.50
1:A:151:PHE:CD1	1:A:151:PHE:C	2.89	0.50
1:A:196:ASN:HD21	1:A:198:ALA:HB3	1.76	0.50
1:A:510:ILE:O	1:A:514:GLN:HG3	2.11	0.50
1:A:294:GLN:H	1:A:297:HIS:CD2	2.20	0.50
1:A:194:VAL:CG1	1:A:195:MET:HE2	2.29	0.50
1:B:208:THR:HG21	1:B:477:ARG:HH12	1.77	0.50
1:A:968:VAL:O	1:A:969:VAL:CG2	2.59	0.49
1:B:968:VAL:HG23	1:B:969:VAL:HG22	1.92	0.49
1:B:733:ILE:HD13	1:B:733:ILE:N	2.28	0.49
1:A:90:LEU:HD13	1:A:169:PHE:CE2	2.48	0.49
1:A:374:ILE:HD11	2:C:3:GLU:HG3	1.94	0.49
1:B:783:ASN:ND2	1:B:785:VAL:H	2.10	0.49
1:A:538:LEU:CD1	1:A:538:LEU:H	2.25	0.49
1:A:722:ARG:HG3	1:A:722:ARG:HH11	1.77	0.49
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.94	0.49
1:A:309:ASP:N	1:A:672:ASN:HD21	1.96	0.49
1:A:429:ARG:HH11	1:A:429:ARG:CB	2.24	0.49
1:A:659:PHE:CE1	1:A:712:LEU:HD12	2.48	0.49
1:B:510:ILE:O	1:B:514:GLN:HG3	2.13	0.49
1:A:374:ILE:HD12	1:A:374:ILE:C	2.38	0.49
1:A:798:ASP:CG	1:A:799:MET:H	2.21	0.49
1:A:49:ARG:HH12	1:A:446:LEU:HD23	1.77	0.49
1:A:135:ALA:HA	1:A:892:ARG:CZ	2.42	0.49
1:A:862:ARG:HA	1:A:862:ARG:NE	2.28	0.48
1:A:864:GLU:HG3	4:A:2301:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:HIS:ND1	1:B:292:PRO:HD2	2.28	0.48
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.94	0.48
1:A:359:LEU:HD23	1:A:360:VAL:N	2.28	0.48
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.14	0.48
1:A:306:PRO:HB3	1:A:481:VAL:CG1	2.44	0.48
1:B:363:GLN:CD	1:B:371:MET:HE1	2.39	0.48
1:B:874:ILE:HG22	1:B:937:ILE:HD11	1.96	0.48
1:B:90:LEU:C	1:B:90:LEU:HD23	2.39	0.48
1:A:538:LEU:HD23	1:A:734:THR:HG23	1.94	0.47
1:A:719:LEU:HD13	1:A:719:LEU:C	2.39	0.47
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.96	0.47
1:A:446:LEU:HD23	4:A:2165:HOH:O	2.09	0.47
1:B:100:PRO:HB2	1:B:102:ASN:ND2	2.29	0.47
1:B:224:TYR:CE2	1:B:229:ARG:HD2	2.48	0.47
1:A:67:LEU:HD23	1:A:67:LEU:N	2.29	0.47
1:A:532:PRO:HG3	1:A:634:TYR:CD2	2.49	0.47
1:A:776:TRP:HA	1:A:953:LYS:O	2.14	0.47
1:A:45:PRO:HG2	1:A:46:ALA:H	1.80	0.47
1:A:568:PHE:HA	4:A:2222:HOH:O	2.13	0.47
1:B:559:LEU:HD11	1:B:729:LEU:HD22	1.95	0.47
1:B:607:TYR:CE2	1:B:644:LYS:HG2	2.49	0.47
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.95	0.47
1:A:196:ASN:HD22	1:A:199:TRP:H	1.60	0.47
1:A:488:LYS:HD3	1:A:488:LYS:N	2.29	0.47
1:A:622:ASN:H	1:A:622:ASN:ND2	2.12	0.47
1:B:184:ASN:HD21	1:B:223:LYS:NZ	2.12	0.47
1:A:102:ASN:N	1:A:102:ASN:ND2	2.57	0.47
1:A:252:ASN:HB3	1:A:280:ASN:OD1	2.15	0.47
1:B:552:LYS:NZ	1:B:743:GLN:NE2	2.62	0.47
1:A:64:TYR:CE2	1:A:450:LEU:HD21	2.49	0.47
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.28	0.47
1:B:298:LEU:HD13	1:B:475:ASN:HA	1.96	0.47
1:B:933:LYS:O	1:B:937:ILE:HG12	2.15	0.47
1:A:879:GLU:OE1	1:A:879:GLU:HA	2.13	0.46
1:B:552:LYS:HZ1	1:B:743:GLN:HE22	1.61	0.46
1:A:843:ILE:HG22	1:A:844:GLN:N	2.30	0.46
1:B:506:PRO:HG2	1:B:509:VAL:CG2	2.46	0.46
1:B:556:MET:O	1:B:556:MET:HG3	2.16	0.46
1:A:768:GLU:HB3	1:A:843:ILE:HG13	1.97	0.46
1:B:501:LYS:HE3	4:B:2166:HOH:O	2.15	0.46
1:B:597:LEU:HG	1:B:620:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:GLN:HB2	1:B:639:PRO:HD3	1.98	0.46
1:B:93:HIS:HD2	1:B:145:GLU:O	1.98	0.46
1:B:404:GLU:HG2	1:B:524:LEU:CD2	2.46	0.46
1:A:90:LEU:HD23	1:A:90:LEU:C	2.41	0.46
1:B:577:GLU:CD	1:B:912:ILE:HD13	2.41	0.46
1:B:151:PHE:CD1	1:B:151:PHE:C	2.94	0.46
1:B:285:LEU:HD22	1:B:286:PRO:HD2	1.98	0.46
1:B:843:ILE:HG22	1:B:844:GLN:N	2.31	0.46
1:B:311:ARG:HD2	1:B:379:LEU:O	2.16	0.46
1:B:67:LEU:HD13	1:B:75:VAL:HB	1.98	0.45
1:B:374:ILE:C	1:B:374:ILE:HD12	2.41	0.45
1:A:357:ASN:HB2	1:A:378:ASP:OD1	2.16	0.45
1:B:204:LEU:HD13	3:B:2001:DIO:H2'2	1.98	0.45
1:A:599:LEU:HD21	1:A:659:PHE:HA	1.99	0.45
1:B:722:ARG:HD2	1:B:756:LYS:HB2	1.98	0.45
1:A:49:ARG:HH22	1:A:446:LEU:HD21	1.81	0.45
1:A:129:GLN:O	1:A:133:GLU:HG3	2.17	0.45
1:A:349:GLU:O	1:A:353:LYS:HG3	2.16	0.45
1:A:517:ASP:OD2	1:A:517:ASP:C	2.58	0.45
1:A:618:TYR:HA	1:A:630:SER:O	2.16	0.45
1:B:529:GLU:O	1:B:637:LYS:HE3	2.17	0.45
1:A:776:TRP:CE3	1:A:989:PRO:HB3	2.52	0.45
1:B:787:ASN:OD1	1:B:962:GLU:HB2	2.17	0.45
1:A:643:LYS:HE3	1:A:647:GLU:OE2	2.17	0.45
1:B:224:TYR:OH	1:B:229:ARG:NH1	2.50	0.45
1:B:886:ILE:HG23	1:B:928:LEU:HD11	1.98	0.45
1:A:227:GLU:C	1:A:230:PRO:HD2	2.42	0.45
1:A:446:LEU:HD22	1:A:446:LEU:N	2.28	0.44
1:A:153:VAL:HG22	1:A:154:SER:N	2.32	0.44
1:A:957:HIS:HD2	4:A:2281:HOH:O	2.00	0.44
1:B:824:ARG:O	1:B:828:GLN:HA	2.16	0.44
1:A:460:ARG:HH12	1:A:462:ASP:CG	2.24	0.44
1:A:796:GLN:HB3	1:A:952:HIS:HB2	2.00	0.44
1:A:815:ILE:HG22	1:A:870:MET:CE	2.47	0.44
1:B:94:ILE:HD12	1:B:248:TYR:CB	2.47	0.44
1:B:567:PHE:HE1	1:B:903:GLU:OE2	1.99	0.44
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.99	0.44
1:A:684:TYR:CZ	1:A:688:LEU:HD11	2.53	0.44
1:B:474:GLU:HG2	1:B:475:ASN:ND2	2.32	0.44
1:B:530:PHE:HA	1:B:637:LYS:HD2	1.99	0.44
1:A:446:LEU:H	1:A:446:LEU:CD2	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:GLN:HE21	1:A:891:ILE:HD11	1.82	0.44
1:A:245:HIS:O	1:A:249:TYR:HB2	2.18	0.44
1:B:591:ASN:O	1:B:595:LEU:CD2	2.60	0.44
1:A:393:HIS:HE1	4:A:2144:HOH:O	2.00	0.44
1:A:418:ASN:HB3	1:A:454:TYR:O	2.18	0.44
1:A:654:ILE:HD13	1:A:712:LEU:HD13	1.98	0.44
1:A:64:TYR:HD2	1:A:76:LEU:HD11	1.83	0.43
1:A:799:MET:HE2	1:A:799:MET:HB2	1.76	0.43
1:B:709:LEU:HG	1:B:713:LYS:HE3	2.00	0.43
1:B:810:LEU:HG	1:B:928:LEU:HD21	1.99	0.43
1:A:346:LEU:HA	1:A:522:PHE:CE2	2.53	0.43
1:B:259:LEU:C	1:B:259:LEU:CD1	2.91	0.43
1:B:577:GLU:CD	1:B:912:ILE:CD1	2.91	0.43
1:A:871:GLU:O	1:A:875:GLU:HG3	2.18	0.43
1:A:908:TRP:CE2	1:A:912:ILE:HD11	2.54	0.43
1:B:799:MET:SD	1:B:1006:PRO:HG2	2.58	0.43
1:A:229:ARG:HB3	1:A:230:PRO:HD3	2.01	0.43
1:B:934:GLU:HG2	1:B:938:LYS:HE2	2.01	0.43
1:A:196:ASN:ND2	1:A:199:TRP:H	2.17	0.43
1:B:400:LYS:HD3	4:B:2146:HOH:O	2.18	0.43
1:B:542:LYS:HG2	1:B:543:GLU:OE2	2.19	0.43
1:B:776:TRP:CE3	1:B:989:PRO:HB3	2.53	0.43
1:B:950:ARG:CD	4:B:2213:HOH:O	2.54	0.43
1:A:196:ASN:ND2	1:A:198:ALA:H	2.16	0.43
1:B:54:ILE:HG22	1:B:450:LEU:HD22	2.01	0.43
1:B:123:LYS:HB3	1:B:126:GLU:HB2	2.01	0.43
1:B:229:ARG:HB3	1:B:230:PRO:CD	2.48	0.43
1:B:767:ARG:NH1	1:B:1006:PRO:HA	2.34	0.43
1:A:654:ILE:HD11	1:A:712:LEU:HD22	2.00	0.43
1:B:88:ALA:HA	1:B:257:CYS:O	2.19	0.43
1:B:353:LYS:HD3	1:B:355:TRP:CZ3	2.54	0.43
1:A:158:LEU:HD23	1:A:158:LEU:O	2.19	0.42
1:A:596:TYR:CD2	1:A:597:LEU:HD13	2.54	0.42
1:B:309:ASP:O	1:B:668:ARG:HG2	2.19	0.42
1:B:460:ARG:HD2	1:B:462:ASP:OD2	2.19	0.42
1:A:794:TYR:CE1	1:A:838:ARG:HD3	2.55	0.42
1:B:860:GLU:OE1	1:B:953:LYS:HE2	2.20	0.42
2:C:16:LYS:HZ2	2:C:16:LYS:HG2	1.57	0.42
1:A:472:ARG:HG2	1:A:472:ARG:HH11	1.84	0.42
1:A:542:LYS:HG3	1:A:543:GLU:HG3	2.01	0.42
1:A:683:MET:HA	1:A:792:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:LEU:HD23	1:A:712:LEU:O	2.20	0.42
1:A:896:LYS:HA	1:A:896:LYS:HD3	1.84	0.42
1:B:208:THR:CG2	1:B:477:ARG:HH12	2.31	0.42
1:B:783:ASN:HD21	1:B:786:HIS:H	1.60	0.42
1:A:793:ILE:O	1:A:847:ARG:HA	2.20	0.42
1:B:306:PRO:HB3	1:B:481:VAL:CG1	2.49	0.42
1:B:398:ILE:HG23	1:B:468:LEU:CD2	2.50	0.42
1:A:392:LEU:O	1:A:396:GLN:HG3	2.19	0.42
1:A:894:LEU:HG	1:A:925:VAL:HG21	2.02	0.42
1:B:404:GLU:HG2	1:B:524:LEU:HD21	2.02	0.42
1:B:446:LEU:HD23	4:B:2269:HOH:O	2.18	0.42
1:A:170:LEU:HD21	1:A:277:GLU:HG3	2.01	0.42
1:A:1009:LYS:HA	1:A:1010:PRO:HD3	1.86	0.42
1:A:842:GLY:HA3	1:A:1008:VAL:HG23	2.02	0.41
1:B:189:GLU:O	1:B:192:LYS:HD2	2.20	0.41
1:B:437:ILE:HA	1:B:440:ILE:HG12	2.02	0.41
1:B:488:LYS:N	1:B:488:LYS:HD3	2.35	0.41
1:B:618:TYR:HA	1:B:630:SER:O	2.20	0.41
1:A:386:HIS:HD2	1:A:389:ASP:OD2	2.03	0.41
1:A:479:ALA:HB2	3:A:2000:DIO:H12	2.02	0.41
1:A:550:LEU:HD11	1:A:558:LYS:HG3	2.01	0.41
1:B:378:ASP:OD2	1:B:378:ASP:C	2.63	0.41
1:B:689:LEU:CD1	1:B:995:MET:HG2	2.50	0.41
1:A:817:GLU:HG3	1:A:818:PRO:CD	2.50	0.41
1:A:337:LEU:HD23	1:A:401:LEU:CD2	2.48	0.41
1:A:634:TYR:O	1:A:638:GLN:HG3	2.21	0.41
1:A:709:LEU:HG	1:A:713:LYS:HE3	2.03	0.41
1:B:179:LYS:HD2	1:B:237:VAL:HB	2.01	0.41
1:B:765:ARG:HD3	1:B:914:GLN:OE1	2.20	0.41
1:B:855:PRO:HB2	1:B:857:HIS:CE1	2.55	0.41
1:A:400:LYS:HD3	4:A:2155:HOH:O	2.19	0.41
1:A:829:LEU:O	1:A:852:SER:HB2	2.21	0.41
1:B:600:LEU:HD23	1:B:620:LEU:HD21	2.02	0.41
1:A:196:ASN:ND2	1:A:198:ALA:N	2.68	0.41
1:A:1003:PRO:HB3	1:B:1006:PRO:HD3	2.03	0.41
1:B:793:ILE:O	1:B:847:ARG:HA	2.20	0.41
1:B:796:GLN:HB3	1:B:952:HIS:HB2	2.02	0.41
1:A:697:LYS:O	1:A:701:LYS:HG2	2.21	0.41
1:A:817:GLU:HG3	1:A:818:PRO:HD3	2.03	0.41
1:B:714:ALA:O	1:B:717:PRO:HD2	2.20	0.41
1:B:965:SER:O	1:B:966:CYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:PRO:HA	1:A:101:PRO:HD3	1.95	0.41
1:B:543:GLU:H	1:B:543:GLU:CD	2.29	0.41
1:B:908:TRP:CZ2	1:B:912:ILE:HD11	2.55	0.41
1:A:90:LEU:HD13	1:A:169:PHE:CD2	2.55	0.41
1:A:279:GLU:HB3	1:A:281:LYS:HE3	2.02	0.41
1:A:559:LEU:HD11	1:A:729:LEU:HG	2.03	0.41
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.56	0.40
1:A:460:ARG:NH1	1:A:462:ASP:CG	2.79	0.40
1:A:776:TRP:CD2	1:A:989:PRO:HB3	2.56	0.40
1:B:196:ASN:ND2	1:B:198:ALA:HB3	2.36	0.40
1:B:208:THR:CG2	1:B:477:ARG:HH22	2.14	0.40
1:B:259:LEU:HD12	1:B:260:GLY:N	2.36	0.40
1:B:552:LYS:HZ1	1:B:743:GLN:NE2	2.20	0.40
1:B:580:SER:HA	1:B:581:PRO:HD3	1.90	0.40
1:B:600:LEU:HD21	1:B:649:MET:CG	2.51	0.40
1:B:843:ILE:HG22	1:B:844:GLN:H	1.86	0.40
1:A:423:ARG:NE	4:A:2544:HOH:O	2.53	0.40
1:A:855:PRO:HA	1:A:856:PRO:HD3	1.90	0.40
1:B:512:LYS:HE3	1:B:512:LYS:HB2	1.85	0.40
1:B:600:LEU:CD2	1:B:649:MET:HG2	2.52	0.40
1:A:250:SER:O	1:A:254:MET:HG3	2.21	0.40
1:B:986:LEU:HA	1:B:987:PRO:HD3	1.94	0.40
1:A:420:VAL:HG12	1:A:634:TYR:OH	2.21	0.40
1:A:824:ARG:O	1:A:828:GLN:HA	2.22	0.40
1:B:86:SER:HB3	1:B:158:LEU:HG	2.03	0.40
1:B:153:VAL:HG22	1:B:154:SER:N	2.36	0.40
1:B:815:ILE:C	1:B:818:PRO:HD2	2.47	0.40
1:A:196:ASN:HD22	1:A:196:ASN:C	2.29	0.40
1:B:94:ILE:HD12	1:B:248:TYR:HB3	2.02	0.40
1:B:120:LYS:HD3	1:B:167:GLN:CD	2.46	0.40
1:B:580:SER:HB2	1:B:723:LEU:HD23	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLN:OE1	1:B:234:GLY:O[5_554]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	960/990 (97%)	927 (97%)	33 (3%)	0	100	100
1	B	961/990 (97%)	934 (97%)	26 (3%)	1 (0%)	48	50
2	C	7/40 (18%)	7 (100%)	0	0	100	100
2	D	7/40 (18%)	7 (100%)	0	0	100	100
All	All	1935/2060 (94%)	1875 (97%)	59 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1012	ILE

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	855/883 (97%)	799 (94%)	56 (6%)	15	13
1	B	854/883 (97%)	790 (92%)	64 (8%)	12	10
2	C	8/31 (26%)	6 (75%)	2 (25%)	0	0
2	D	9/31 (29%)	6 (67%)	3 (33%)	0	0
All	All	1726/1828 (94%)	1601 (93%)	125 (7%)	13	11

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	97	LEU
1	A	102	ASN
1	A	119	LYS
1	A	125	ASN
1	A	158	LEU
1	A	179	LYS
1	A	196	ASN
1	A	201	LEU
1	A	226	LEU
1	A	238	ARG
1	A	270	LEU
1	A	285	LEU
1	A	337	LEU
1	A	347	LEU
1	A	356	VAL
1	A	417	LEU
1	A	425	LYS
1	A	429	ARG
1	A	450	LEU
1	A	454	TYR
1	A	466	MET
1	A	475	ASN
1	A	488	LYS
1	A	524	LEU
1	A	542	LYS
1	A	543	GLU
1	A	558	LYS
1	A	595	LEU
1	A	597	LEU
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	642	LEU
1	A	648	LYS
1	A	657	LYS
1	A	722	ARG
1	A	728	LEU
1	A	733	ILE
1	A	756	LYS
1	A	771	LEU
1	A	783	ASN
1	A	788	ASN

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Mol	Chain	Res	Type
1	A	799	MET
1	A	810	LEU
1	A	823	LEU
1	A	846	LEU
1	A	859	LEU
1	A	860	GLU
1	A	867	LEU
1	A	879	GLU
1	A	880	GLU
1	A	889	LEU
1	A	928	LEU
1	A	969	VAL
1	A	1007	LEU
1	B	48	LYS
1	B	67	LEU
1	B	94	ILE
1	B	97	LEU
1	B	102	ASN
1	B	116	LEU
1	B	125	ASN
1	B	158	LEU
1	B	162	LEU
1	B	173	LEU
1	B	192	LYS
1	B	201	LEU
1	B	204	LEU
1	B	208	THR
1	B	226	LEU
1	B	256	VAL
1	B	259	LEU
1	B	324	LYS
1	B	337	LEU
1	B	417	LEU
1	B	425	LYS
1	B	450	LEU
1	B	468	LEU
1	B	470	LYS
1	B	488	LYS
1	B	543	GLU
1	B	556	MET
1	B	597	LEU
1	B	598	GLU

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Mol	Chain	Res	Type
1	B	613	LEU
1	B	616	LEU
1	B	621	GLN
1	B	622	ASN
1	B	629	LEU
1	B	642	LEU
1	B	657	LYS
1	B	668	ARG
1	B	689	LEU
1	B	700	LEU
1	B	701	LYS
1	B	712	LEU
1	B	719	LEU
1	B	720	LEU
1	B	728	LEU
1	B	733	ILE
1	B	756	LYS
1	B	771	LEU
1	B	781	GLN
1	B	788	ASN
1	B	810	LEU
1	B	817	GLU
1	B	823	LEU
1	B	846	LEU
1	B	859	LEU
1	B	861	SER
1	B	889	LEU
1	B	896	LYS
1	B	928	LEU
1	B	938	LYS
1	B	962	GLU
1	B	969	VAL
1	B	981	SER
1	B	993	GLN
1	B	1002	LEU
2	C	3	GLU
2	C	23	ASP
2	D	3	GLU
2	D	17	LEU
2	D	22	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) 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	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	376	ASN
1	A	386	HIS
1	A	393	HIS
1	A	407	GLN
1	A	412	GLN
1	A	475	ASN
1	A	499	GLN
1	A	502	GLN
1	A	575	ASN
1	A	621	GLN
1	A	622	ASN
1	A	672	ASN
1	A	718	GLN
1	A	730	HIS
1	A	736	GLN
1	A	752	HIS
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	887	GLN
1	A	922	ASN
1	A	957	HIS
1	B	93	HIS
1	B	102	ASN
1	B	125	ASN
1	B	129	GLN
1	B	157	HIS
1	B	184	ASN
1	B	196	ASN
1	B	232	GLN
1	B	294	GLN
1	B	297	HIS

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Mol	Chain	Res	Type
1	B	300	GLN
1	B	332	HIS
1	B	376	ASN
1	B	399	GLN
1	B	475	ASN
1	B	499	GLN
1	B	502	GLN
1	B	621	GLN
1	B	622	ASN
1	B	672	ASN
1	B	679	HIS
1	B	718	GLN
1	B	730	HIS
1	B	732	ASN
1	B	743	GLN
1	B	752	HIS
1	B	770	GLN
1	B	781	GLN
1	B	783	ASN
1	B	805	ASN
1	B	828	GLN
1	B	883	GLN
1	B	922	ASN
1	B	957	HIS
1	B	993	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	B	2001	-	6,6,6	0.84	0	6,6,6	0.23	0
3	DIO	A	2000	-	6,6,6	0.79	0	6,6,6	0.24	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	B	2001	-	-	-	0/1/1/1
3	DIO	A	2000	-	-	-	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	DIO	2	0
3	A	2000	DIO	1	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	964/990 (97%)	0.29	40 (4%) 41 43	22, 34, 50, 71	0
1	B	965/990 (97%)	0.14	36 (3%) 45 47	18, 30, 48, 74	0
2	C	11/40 (27%)	1.95	6 (54%) 0 0	38, 45, 51, 56	0
2	D	11/40 (27%)	1.72	2 (18%) 3 3	33, 41, 50, 51	0
All	All	1951/2060 (94%)	0.23	84 (4%) 40 41	18, 32, 50, 74	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1012	ILE	8.0
1	B	1014	PHE	7.5
1	A	1016	ALA	6.2
1	A	964	ASP	6.1
1	A	1012	ILE	5.9
1	B	44	ASN	5.6
1	A	45	PRO	5.5
1	A	1014	PHE	5.4
1	A	979	ASN	5.3
1	B	1011	HIS	5.1
1	B	979	ASN	5.0
1	A	969	VAL	5.0
1	A	1011	HIS	4.7
1	A	970	GLY	4.3
1	B	764	VAL	4.1
1	A	706	ASP	4.1
1	B	964	ASP	4.0
1	B	978	ILE	4.0
1	B	765	ARG	4.0
1	A	475	ASN	3.8
1	A	1015	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	970	GLY	3.8
1	B	971	GLU	3.5
1	A	1013	ASN	3.3
1	B	763	LEU	3.3
2	D	23	ASP	3.3
1	A	968	VAL	3.2
1	A	53	HIS	3.1
1	B	702	GLU	3.1
1	A	965	SER	3.1
1	A	871	GLU	2.9
1	B	969	VAL	2.9
1	B	782	ARG	2.9
1	B	982	GLN	2.8
2	C	17	LEU	2.8
1	A	896	LYS	2.8
1	B	759	LEU	2.8
1	A	966	CYS	2.8
1	B	981	SER	2.8
1	A	993	GLN	2.7
1	A	963	MET	2.7
2	D	22	GLU	2.7
1	A	930	THR	2.7
1	A	454	TYR	2.7
1	A	967	PRO	2.7
1	B	295	GLU	2.7
1	A	508	GLU	2.6
1	A	47	ILE	2.6
1	A	980	LEU	2.5
2	C	19	PHE	2.5
2	C	18	VAL	2.4
1	B	352	SER	2.4
1	B	968	VAL	2.4
2	C	23	ASP	2.4
1	B	543	GLU	2.4
1	B	962	GLU	2.3
1	A	517	ASP	2.3
1	B	625	TYR	2.3
1	A	938	LYS	2.3
1	B	965	SER	2.3
2	C	21	ALA	2.2
1	A	295	GLU	2.2
1	B	517	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	239	GLN	2.2
1	B	94	ILE	2.2
1	B	492	THR	2.2
1	B	705	ASP	2.2
1	A	287	GLU	2.2
1	A	458	GLU	2.2
1	B	234	GLY	2.2
1	B	577	GLU	2.2
1	B	208	THR	2.2
1	A	880	GLU	2.1
1	A	934	GLU	2.1
1	B	510	ILE	2.1
1	B	555	ALA	2.1
1	A	67	LEU	2.1
2	C	3	GLU	2.1
1	B	1010	PRO	2.1
1	A	764	VAL	2.1
1	A	705	ASP	2.1
1	A	711	ARG	2.1
1	B	934	GLU	2.0
1	A	52	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DIO	B	2001	6/6	0.90	0.16	52,52,53,53	0
3	DIO	A	2000	6/6	0.93	0.17	55,56,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.