



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:51 AM UTC

PDB ID : 1J79 / pdb_00001j79
Title : Molecular Structure of Dihydroorotase: A Paradigm for Catalysis Through the Use of a Binuclear Metal Center
Authors : Thoden, J.B.; Phillips Jr., G.N.; Neal, T.M.; Raushel, F.M.; Holden, H.M.
Deposited on : 2001-05-16
Resolution : 1.70 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

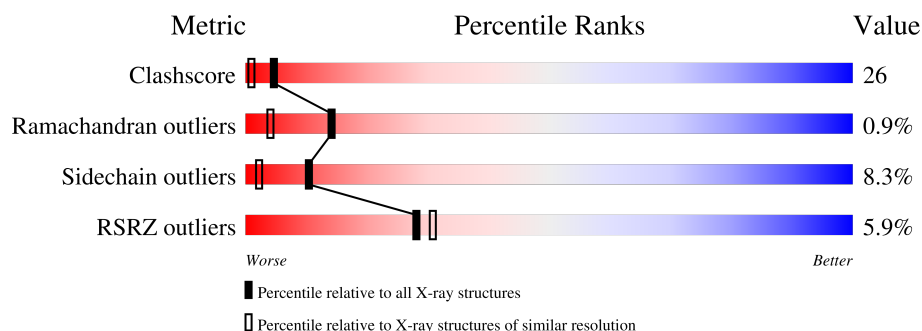
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	347	3% 59% 31% 7% ..
1	B	347	8% 54% 35% 7% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6212 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 dihydroorotase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	11	0
			2751	1742	491	502	16			
1	B	339	Total	C	N	O	S	0	3	0
			2691	1703	479	493	16			

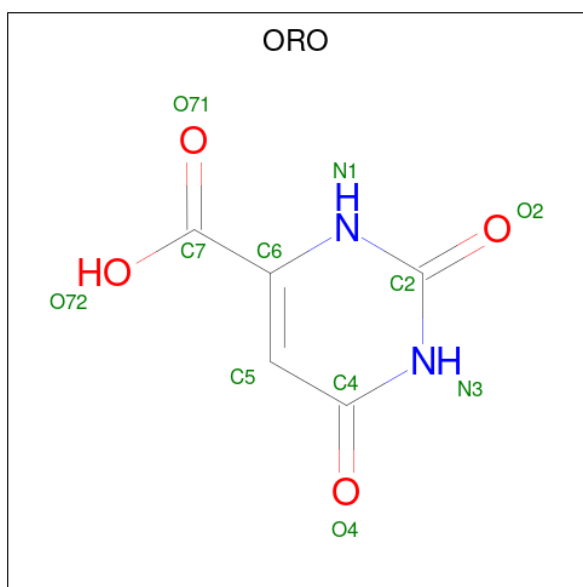
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	PRO	GLY	SEE REMARK 999	UNP P05020
A	102	KCX	LYS	modified residue	UNP P05020
A	119	VAL	ILE	SEE REMARK 999	UNP P05020
A	243	GLN	ASN	SEE REMARK 999	UNP P05020
B	69	PRO	GLY	SEE REMARK 999	UNP P05020
B	102	KCX	LYS	modified residue	UNP P05020
B	119	VAL	ILE	SEE REMARK 999	UNP P05020
B	243	GLN	ASN	SEE REMARK 999	UNP P05020

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

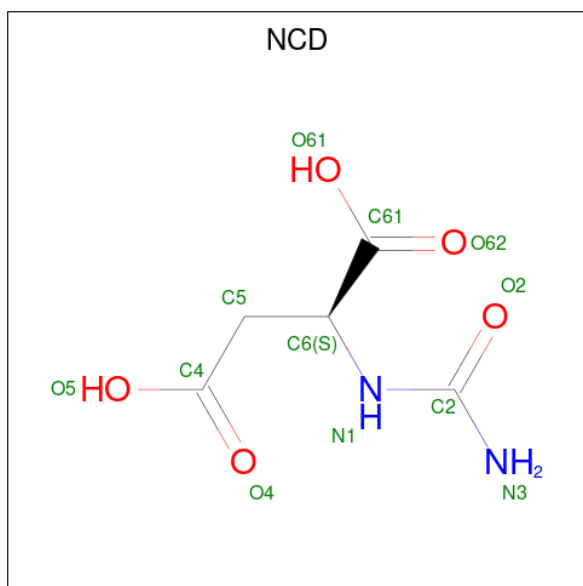
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is OROTIC ACID (CCD ID: ORO) (formula: C₅H₄N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	2	4		

- Molecule 4 is N-CARBAMOYL-L-ASPARTATE (CCD ID: NCD) (formula: $C_5H_8N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	5	2	5		
4	B	1	Total	C	N	O	0	0
			12	5	2	5		

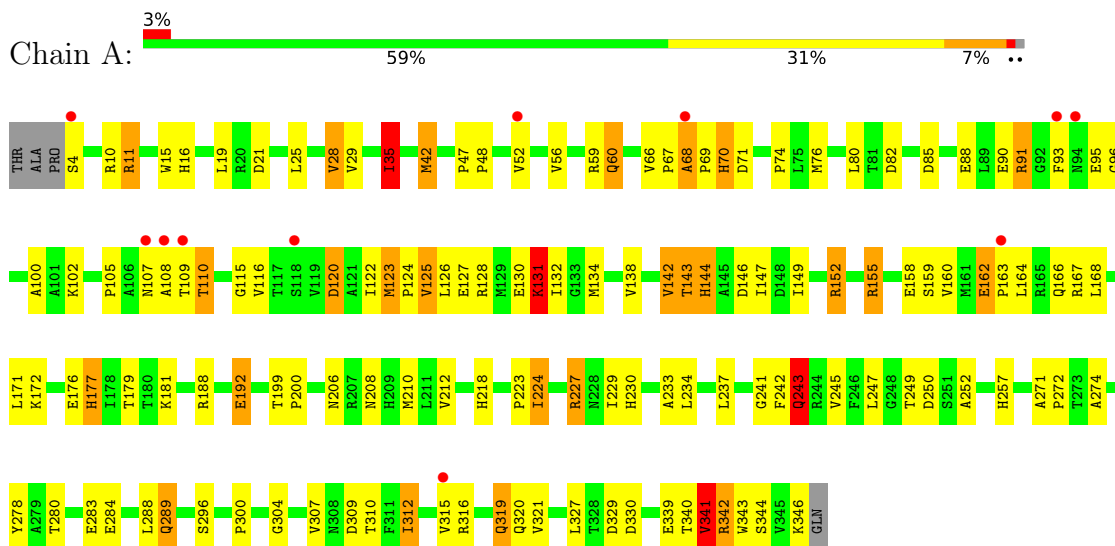
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	413	Total 413	O 413	0	0
5	B	318	Total 318	O 318	0	0

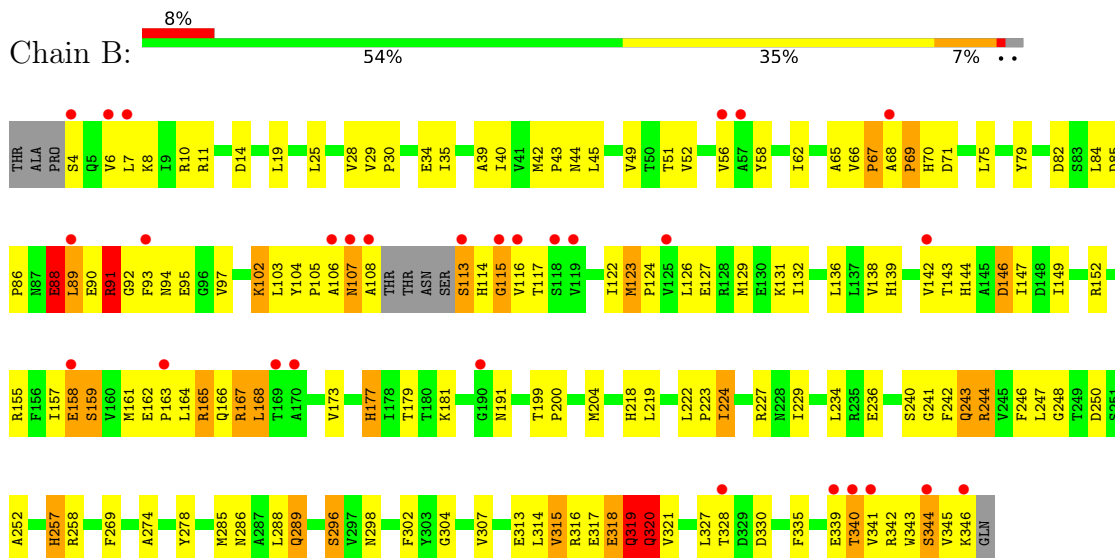
3 Residue-property plots

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: dihydroorotase



• Molecule 1: dihydroorotase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.60Å 78.80Å 180.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 30.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.70) 96.6 (30.00-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.80 (at 1.50Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.191 , 0.258 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 123.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6212	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 4.68% 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: ORO, ZN, NCD, KCX

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	1.10	0/2845	1.50	34/3869 (0.9%)
1	B	1.07	0/2752	1.51	31/3740 (0.8%)
All	All	1.08	0/5597	1.51	65/7609 (0.9%)

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ILE	N-CA-C	9.79	119.97	111.56
1	B	28	VAL	N-CA-C	7.87	119.58	111.00
1	A	166	GLN	CB-CA-C	7.83	124.16	110.85
1	B	146	ASP	N-CA-CB	7.43	121.90	110.46
1	B	257	HIS	CA-CB-CG	-7.40	106.40	113.80
1	B	138	VAL	N-CA-C	7.38	118.44	108.11
1	A	252	ALA	N-CA-CB	-7.26	102.09	111.09
1	B	168	LEU	CA-C-N	7.01	129.98	120.38
1	B	168	LEU	C-N-CA	7.01	129.98	120.38
1	A	35	ILE	CB-CA-C	-6.94	104.85	111.44
1	A	342	ARG	N-CA-C	6.89	118.45	111.07
1	A	144	HIS	CA-CB-CG	-6.85	106.95	113.80
1	B	224	ILE	N-CA-C	6.74	119.14	109.51
1	A	152	ARG	N-CA-C	6.60	118.47	111.28
1	B	296	SER	N-CA-CB	-6.48	102.43	110.98
1	A	227	ARG	N-CA-CB	6.39	119.50	110.36
1	A	146	ASP	CA-C-N	-6.26	115.04	122.93
1	A	146	ASP	C-N-CA	-6.26	115.04	122.93
1	B	173	VAL	N-CA-C	6.26	117.13	108.12
1	B	321	VAL	N-CA-C	6.21	116.87	108.17
1	B	258	ARG	N-CA-C	-6.20	105.54	113.23
1	A	35	ILE	N-CA-CB	-6.00	104.81	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	ARG	N-CA-C	6.00	118.61	111.71
1	A	143	THR	N-CA-C	5.98	119.53	112.72
1	B	274	ALA	N-CA-C	5.97	118.31	111.02
1	A	138	VAL	N-CA-C	5.83	116.28	108.11
1	A	243	GLN	CA-CB-CG	-5.82	102.46	114.10
1	B	69	PRO	N-CA-C	5.82	121.20	113.40
1	B	88	GLU	N-CA-C	-5.78	104.95	112.23
1	B	269	PHE	CA-CB-CG	-5.76	108.04	113.80
1	B	252	ALA	CA-C-N	5.75	125.51	119.76
1	B	252	ALA	C-N-CA	5.75	125.51	119.76
1	B	67	PRO	N-CA-CB	5.67	108.08	103.32
1	A	131[A]	LYS	N-CA-C	5.66	117.13	111.07
1	A	131[B]	LYS	N-CA-C	5.66	117.13	111.07
1	B	240	SER	CA-C-N	-5.60	113.72	122.51
1	B	240	SER	C-N-CA	-5.60	113.72	122.51
1	A	218	HIS	CA-CB-CG	-5.58	108.22	113.80
1	A	28	VAL	N-CA-C	5.50	118.81	111.44
1	A	76	MET	N-CA-C	5.46	117.92	110.55
1	B	218	HIS	CA-CB-CG	-5.42	108.39	113.80
1	B	88	GLU	CA-C-O	5.41	126.17	119.79
1	B	319	GLN	N-CA-CB	5.40	119.43	110.63
1	B	320	GLN	N-CA-C	5.36	118.84	110.32
1	A	42	MET	CB-CA-C	5.31	117.81	109.27
1	A	341	VAL	N-CA-CB	-5.28	104.65	110.99
1	A	329	ASP	N-CA-C	5.28	119.69	112.88
1	A	274	ALA	N-CA-C	5.27	116.70	111.07
1	B	45	LEU	CA-C-N	-5.24	116.09	122.64
1	B	45	LEU	C-N-CA	-5.24	116.09	122.64
1	A	250	ASP	N-CA-CB	5.23	120.25	112.30
1	A	249	THR	N-CA-C	5.22	116.97	111.28
1	A	159	SER	CA-C-N	-5.19	117.66	123.16
1	A	159	SER	C-N-CA	-5.19	117.66	123.16
1	A	110	THR	N-CA-C	5.19	117.74	109.96
1	A	160	VAL	N-CA-C	5.12	115.67	111.62
1	B	320	GLN	N-CA-CB	-5.11	102.09	110.41
1	A	70	HIS	N-CA-C	5.09	117.94	110.30
1	A	341	VAL	CA-C-N	5.07	127.03	120.44
1	A	341	VAL	C-N-CA	5.07	127.03	120.44
1	B	227	ARG	N-CA-CB	-5.03	102.64	110.04
1	A	142[A]	VAL	N-CA-C	-5.02	101.18	108.36
1	A	142[B]	VAL	N-CA-C	-5.02	101.18	108.36
1	B	250	ASP	N-CA-C	-5.02	107.11	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	GLY	N-CA-C	-5.01	101.30	113.18

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	2751	0	2725	126	0
1	B	2691	0	2658	153	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	11	0	3	0	0
4	A	12	0	6	5	0
4	B	12	0	6	2	0
5	A	413	0	0	11	1
5	B	318	0	0	21	0
All	All	6212	0	5398	282	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 26.

All (282) 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:243:GLN:H	1:B:243:GLN:NE2	1.50	1.10
1:B:29:VAL:HG23	1:B:30:PRO:HD3	1.33	1.04
1:B:6:VAL:HG12	1:B:315:VAL:HG13	1.49	0.95
1:B:319:GLN:HG2	1:B:320:GLN:H	1.38	0.88
1:B:93:PHE:CD2	1:B:132:ILE:HD12	2.10	0.86
1:B:243:GLN:H	1:B:243:GLN:HE21	1.19	0.85
1:B:52:VAL:HG13	1:B:97:VAL:HG21	1.60	0.84
1:A:289:GLN:H	1:A:289:GLN:HE21	1.21	0.84
1:B:68:ALA:HB3	1:B:69:PRO:HD3	1.57	0.84
1:A:212:VAL:HG11	4:A:950:NCD:O62	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142[B]:VAL:HG23	1:A:147:ILE:HD13	1.62	0.81
1:B:123:MET:HE3	1:B:167:ARG:NE	1.96	0.80
1:B:6:VAL:HG12	1:B:315:VAL:CG1	2.11	0.80
1:A:123:MET:HA	1:A:123:MET:HE3	1.64	0.80
1:B:7:LEU:HD11	1:B:288:LEU:HD22	1.65	0.79
1:A:142[B]:VAL:CG2	1:A:147:ILE:HD13	2.14	0.78
1:A:91:ARG:O	1:A:95:GLU:HG3	1.84	0.77
1:B:35:ILE:HD11	1:B:345:VAL:HG11	1.64	0.77
1:B:25:LEU:O	1:B:29:VAL:HG22	1.85	0.77
1:B:123:MET:HE3	1:B:167:ARG:CD	2.15	0.77
1:A:11[A]:ARG:HD2	1:A:310:THR:OG1	1.85	0.76
1:A:96:GLY:C	5:A:1299:HOH:O	2.28	0.76
1:A:316:ARG:HB2	1:A:343:TRP:CZ3	2.21	0.75
1:B:29:VAL:CG2	1:B:30:PRO:HD3	2.14	0.75
1:B:52:VAL:CG1	1:B:97:VAL:HG21	2.15	0.75
1:B:243:GLN:HE21	1:B:243:GLN:N	1.85	0.75
1:B:103:LEU:CD1	1:B:116:VAL:HG21	2.17	0.74
1:B:108:ALA:C	1:B:113:SER:HA	2.11	0.74
1:A:127:GLU:O	1:A:131[A]:LYS:HD3	1.87	0.74
1:A:107[A]:ASN:OD1	1:A:109:THR:HB	1.87	0.73
1:B:316:ARG:NH2	1:B:342:ARG:HD3	2.04	0.73
1:B:84:LEU:HD12	5:B:1185:HOH:O	1.87	0.73
1:B:123:MET:HE3	1:B:167:ARG:CZ	2.19	0.73
1:A:309:ASP:HA	5:A:1213:HOH:O	1.90	0.71
1:A:25[B]:LEU:HD12	1:A:29:VAL:HG23	1.72	0.71
1:A:155[B]:ARG:HG2	5:A:1400:HOH:O	1.90	0.71
1:B:106:ALA:C	1:B:107:ASN:HD22	1.99	0.71
4:B:411:NCD:H31	4:B:411:NCD:C4	2.04	0.70
1:B:243:GLN:NE2	1:B:243:GLN:N	2.34	0.70
1:B:52:VAL:HG22	1:B:92:GLY:HA3	1.73	0.70
1:B:49:VAL:HG22	5:B:1551:HOH:O	1.92	0.69
1:B:122:ILE:HD12	1:B:126:LEU:HD21	1.74	0.69
1:A:208:ASN:HB3	4:A:950:NCD:H61	1.73	0.69
1:A:91:ARG:HD2	1:A:95:GLU:OE2	1.93	0.69
1:A:316:ARG:HB2	1:A:343:TRP:CH2	2.28	0.68
1:A:11[A]:ARG:HE	1:A:312:ILE:HD12	1.57	0.67
1:B:200:PRO:O	1:B:204:MET:HG3	1.94	0.67
1:A:128:ARG:O	1:A:132:ILE:HG12	1.93	0.67
1:B:35:ILE:CD1	1:B:345:VAL:HG11	2.25	0.66
1:B:123:MET:HE3	1:B:167:ARG:HD2	1.77	0.66
1:B:103:LEU:HD11	1:B:116:VAL:HG21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PRO:O	1:B:107:ASN:ND2	2.30	0.65
1:B:85:ASP:O	1:B:88:GLU:HB2	1.97	0.63
1:B:319:GLN:HG2	1:B:320:GLN:N	2.07	0.63
1:A:242:PHE:HD2	1:A:245[B]:VAL:HG13	1.62	0.63
1:B:204:MET:HE3	5:B:1333:HOH:O	1.97	0.63
1:B:91[B]:ARG:HD2	1:B:95:GLU:OE2	1.99	0.62
1:A:68:ALA:HB3	1:A:69:PRO:HD3	1.81	0.62
1:A:188:ARG:NH2	5:A:1519:HOH:O	2.31	0.62
1:A:131[B]:LYS:HD2	5:A:1605:HOH:O	1.98	0.61
1:A:144:HIS:HB2	1:A:147:ILE:HD12	1.83	0.61
1:B:62:ILE:O	1:B:66:VAL:HG23	2.01	0.61
1:A:242:PHE:CD2	1:A:245[B]:VAL:HG13	2.36	0.61
1:A:123:MET:HE3	1:A:123:MET:CA	2.26	0.60
1:A:280:THR:O	1:A:284:GLU:HG3	2.00	0.60
1:A:11[A]:ARG:NE	1:A:312:ILE:HD12	2.16	0.60
1:A:107[B]:ASN:ND2	1:A:110:THR:OG1	2.29	0.59
1:B:162:GLU:HB3	1:B:163:PRO:HD3	1.84	0.59
1:B:313:GLU:OE2	1:B:346:LYS:HE3	2.02	0.59
1:A:315:VAL:HG23	1:A:346:LYS:HB2	1.85	0.59
1:A:164:LEU:CD1	1:A:168:LEU:HD12	2.32	0.59
1:B:25:LEU:HD12	1:B:29:VAL:HG13	1.83	0.58
1:A:90:GLU:OE1	1:A:128:ARG:HD2	2.04	0.58
1:B:142:VAL:CG2	1:B:147:ILE:HD13	2.33	0.58
1:B:302:PHE:HB2	5:B:1323:HOH:O	2.02	0.58
1:B:241:GLY:O	1:B:242:PHE:C	2.47	0.58
1:A:283:GLU:OE1	1:A:342:ARG:NH1	2.29	0.57
1:B:315:VAL:CG2	1:B:346:LYS:HB3	2.34	0.57
1:B:162:GLU:O	1:B:163:PRO:C	2.48	0.56
1:B:236:GLU:OE2	1:B:285:MET:HE1	2.04	0.56
1:B:243:GLN:H	1:B:243:GLN:CD	2.12	0.56
1:B:177:HIS:CE1	1:B:223:PRO:HD3	2.41	0.56
1:A:125:VAL:HG12	1:A:126:LEU:N	2.20	0.56
1:A:164:LEU:HD11	1:A:168:LEU:HD12	1.88	0.56
1:B:90:GLU:O	1:B:94:ASN:N	2.35	0.56
1:B:222:LEU:HA	1:B:223:PRO:C	2.30	0.56
1:B:43:PRO:HB2	1:B:79:TYR:HB2	1.88	0.56
1:B:8:LYS:HG3	1:B:313:GLU:HG3	1.88	0.55
1:B:29:VAL:HG23	1:B:30:PRO:CD	2.22	0.55
1:A:181:LYS:HB2	1:A:233:ALA:CB	2.36	0.55
1:B:144:HIS:N	1:B:147:ILE:HD12	2.22	0.55
1:B:7:LEU:N	1:B:314:LEU:O	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107[B]:ASN:HB2	1:A:110:THR:OG1	2.07	0.54
1:B:144:HIS:HB3	1:B:147:ILE:CD1	2.36	0.54
1:B:161:MET:O	1:B:164:LEU:HB3	2.08	0.54
1:A:319:GLN:O	1:A:341:VAL:N	2.30	0.54
1:B:315:VAL:HG21	1:B:346:LYS:HB3	1.90	0.54
1:B:40:ILE:HD13	1:B:75:LEU:HB2	1.90	0.53
1:A:162:GLU:N	1:A:163:PRO:HD2	2.23	0.53
1:A:237:LEU:HD21	1:A:245[B]:VAL:HG11	1.89	0.53
1:B:90:GLU:O	1:B:93:PHE:HB3	2.09	0.53
1:A:142[B]:VAL:HG21	1:A:147:ILE:HD13	1.91	0.53
1:A:144:HIS:HB2	1:A:147:ILE:CD1	2.39	0.53
1:A:316:ARG:HH21	1:A:342:ARG:HD3	1.72	0.53
1:A:164:LEU:HD11	1:A:168:LEU:CD1	2.39	0.53
1:B:107:ASN:HD22	1:B:107:ASN:N	2.05	0.53
1:B:335:PHE:HD1	5:B:1320:HOH:O	1.92	0.53
1:A:25[B]:LEU:CD1	1:A:29:VAL:HG23	2.38	0.53
1:B:52:VAL:HG22	1:B:92:GLY:CA	2.38	0.53
1:B:167:ARG:O	1:B:167:ARG:HG2	2.08	0.53
1:A:11[B]:ARG:NH1	1:A:71:ASP:O	2.42	0.52
1:B:242:PHE:CZ	1:B:244:ARG:HB2	2.44	0.52
1:A:120:ASP:CG	1:A:167:ARG:HH22	2.16	0.52
1:B:107:ASN:ND2	1:B:143:THR:HG21	2.24	0.52
1:B:165:ARG:NH2	5:B:1448:HOH:O	2.25	0.52
1:B:95:GLU:HB2	1:B:97:VAL:HG23	1.91	0.52
1:A:237:LEU:CD2	1:A:245[B]:VAL:HG11	2.40	0.51
1:B:90:GLU:HG2	1:B:94:ASN:ND2	2.25	0.51
1:A:181:LYS:HB2	1:A:233:ALA:HB2	1.93	0.51
1:B:67:PRO:HG2	1:B:70:HIS:CE1	2.45	0.51
1:B:85:ASP:OD2	1:B:86:PRO:HD2	2.10	0.51
1:A:11[A]:ARG:HG3	1:A:312:ILE:HD13	1.93	0.50
1:A:47:PRO:HB2	1:A:48:PRO:HD2	1.92	0.50
1:A:128:ARG:O	1:A:128:ARG:HG3	2.11	0.50
1:A:179:THR:HA	1:A:234:LEU:HD11	1.93	0.50
1:A:316:ARG:O	1:A:316:ARG:HG2	2.11	0.50
1:A:52:VAL:O	1:A:56:VAL:HG23	2.12	0.49
1:A:210:MET:HE1	1:A:224:ILE:HD11	1.94	0.49
1:A:21:ASP:HA	1:A:25[A]:LEU:HB2	1.94	0.49
1:A:212:VAL:HG22	1:B:149:ILE:HD12	1.95	0.49
1:B:162:GLU:HB3	1:B:163:PRO:CD	2.43	0.49
1:B:327:LEU:O	1:B:328:THR:C	2.55	0.49
1:A:283:GLU:OE2	1:A:316:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLN:HE21	1:A:289:GLN:N	2.01	0.49
1:B:58:TYR:O	1:B:62:ILE:HG13	2.13	0.49
1:B:123:MET:N	1:B:124:PRO:HD2	2.28	0.49
1:B:144:HIS:H	1:B:147:ILE:HD12	1.78	0.49
1:B:162:GLU:OE2	1:B:166:GLN:NE2	2.45	0.49
1:B:6:VAL:HA	1:B:314:LEU:O	2.13	0.48
1:B:25:LEU:CD1	1:B:29:VAL:HG13	2.43	0.48
1:B:122:ILE:C	1:B:124:PRO:HD2	2.38	0.48
1:B:92:GLY:O	1:B:97:VAL:N	2.42	0.48
1:A:70:HIS:N	1:A:70:HIS:CD2	2.80	0.48
1:B:179:THR:CG2	1:B:223:PRO:HG2	2.44	0.48
1:A:35:ILE:HD13	5:A:1494:HOH:O	2.12	0.48
1:A:131[A]:LYS:HE3	5:A:1605:HOH:O	2.12	0.48
1:A:192:GLU:CD	1:A:192:GLU:H	2.22	0.48
1:A:199:THR:HB	1:A:200:PRO:HD2	1.96	0.48
1:A:320:GLN:HA	1:A:339:GLU:O	2.14	0.48
1:B:71:ASP:OD2	5:B:1557:HOH:O	2.20	0.47
4:A:950:NCD:O61	4:A:950:NCD:O5	2.32	0.47
1:B:142:VAL:HG21	1:B:147:ILE:HD13	1.95	0.47
1:B:304:GLY:HA2	5:B:1657:HOH:O	2.15	0.47
1:B:257:HIS:HD2	1:B:330:ASP:CG	2.23	0.47
1:A:16:HIS:CE1	1:A:42:MET:HE3	2.49	0.47
1:B:179:THR:HG23	1:B:223:PRO:HG2	1.97	0.47
1:B:88:GLU:OE1	1:B:88:GLU:HA	2.13	0.47
1:B:90:GLU:HG2	1:B:94:ASN:HD21	1.80	0.47
1:A:247:LEU:HG	1:A:278:TYR:CE1	2.49	0.47
1:B:124:PRO:HG2	5:B:1439:HOH:O	2.15	0.47
1:A:47:PRO:CB	1:A:48:PRO:HD2	2.45	0.47
1:A:229:ILE:HG13	1:A:230:HIS:N	2.29	0.47
1:A:149:ILE:O	1:A:152:ARG:HG3	2.14	0.47
1:B:296:SER:HA	5:B:1096:HOH:O	2.14	0.47
1:B:181:LYS:HE2	5:B:1726:HOH:O	2.15	0.46
1:B:257:HIS:HD2	1:B:330:ASP:OD1	1.97	0.46
1:A:116:VAL:HG22	1:A:122:ILE:HG21	1.96	0.46
1:A:316:ARG:HH21	1:A:342:ARG:CD	2.28	0.46
1:B:123:MET:CE	1:B:167:ARG:HD2	2.44	0.46
1:B:247:LEU:C	1:B:247:LEU:HD23	2.40	0.46
1:A:90:GLU:HG3	1:A:132:ILE:HG21	1.96	0.46
1:B:103:LEU:HD12	1:B:116:VAL:HG21	1.94	0.46
1:A:327:LEU:HB2	1:A:330:ASP:O	2.14	0.46
1:B:7:LEU:HG	1:B:343:TRP:CH2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ALA:HB2	5:B:1641:HOH:O	2.15	0.46
1:B:8:LYS:NZ	5:B:1627:HOH:O	2.29	0.46
1:B:346:LYS:HA	5:B:1583:HOH:O	2.15	0.46
1:A:271:ALA:N	1:A:272:PRO:CD	2.78	0.46
1:A:162:GLU:OE2	1:A:162:GLU:HA	2.16	0.46
1:A:304:GLY:HA2	5:A:1208:HOH:O	2.15	0.45
1:A:123:MET:N	1:A:124:PRO:HD2	2.31	0.45
1:A:100:ALA:C	1:A:134:MET:HE2	2.41	0.45
1:A:15:TRP:CZ2	1:A:300:PRO:HD3	2.51	0.45
1:A:82:ASP:OD1	1:A:116:VAL:HA	2.16	0.45
1:B:162:GLU:HG3	1:B:166:GLN:CD	2.41	0.45
1:A:67:PRO:C	1:A:69:PRO:HD2	2.41	0.45
1:A:130:GLU:HG3	1:A:171:LEU:N	2.31	0.45
1:A:176:GLU:O	1:A:177:HIS:C	2.58	0.45
1:B:102:KCX:CX	1:B:104:TYR:CE2	2.99	0.45
1:A:85:ASP:O	1:A:88:GLU:N	2.42	0.45
1:B:10:ARG:O	1:B:11:ARG:C	2.59	0.45
1:B:68:ALA:HB3	1:B:69:PRO:CD	2.39	0.45
1:B:315:VAL:HG23	1:B:344:SER:O	2.17	0.45
1:A:80:LEU:HD22	1:A:125:VAL:HG11	1.99	0.45
1:B:123:MET:N	1:B:124:PRO:CD	2.79	0.45
1:B:129:MET:HE1	1:B:136:LEU:HD13	1.99	0.45
1:A:123:MET:N	1:A:124:PRO:CD	2.79	0.44
1:B:129:MET:HE2	1:B:129:MET:HB2	1.79	0.44
1:B:155[B]:ARG:HG2	5:B:1562:HOH:O	2.16	0.44
1:B:242:PHE:CZ	1:B:244:ARG:CB	3.00	0.44
1:B:14:ASP:O	1:B:39:ALA:HA	2.17	0.44
1:B:82:ASP:OD2	1:B:117:THR:OG1	2.29	0.44
1:B:127:GLU:HG3	1:B:168:LEU:HD21	1.99	0.44
1:A:11[A]:ARG:NE	1:A:312:ILE:CD1	2.80	0.44
1:A:212:VAL:HB	4:A:950:NCD:N1	2.32	0.44
1:B:289:GLN:H	1:B:289:GLN:HE21	1.63	0.44
1:A:59:ARG:HG3	1:A:74:PRO:HG2	1.99	0.44
1:B:10:ARG:HD3	1:B:307:VAL:HB	1.99	0.44
1:A:257:HIS:ND1	1:A:330:ASP:OD2	2.39	0.44
1:B:341:VAL:HG21	5:B:1475:HOH:O	2.18	0.44
1:A:162:GLU:N	1:A:163:PRO:CD	2.81	0.44
1:B:247:LEU:HG	1:B:278:TYR:CE1	2.53	0.44
1:A:66:VAL:CG1	1:A:70:HIS:HB2	2.48	0.43
1:A:123:MET:HA	1:A:123:MET:CE	2.41	0.43
1:A:123:MET:HE2	1:A:123:MET:HB3	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:950:NCD:C4	5:A:1446:HOH:O	2.66	0.43
1:A:107[A]:ASN:ND2	1:A:108:ALA:N	2.66	0.43
1:B:34:GLU:HG3	1:B:35:ILE:HG12	1.99	0.43
1:B:246:PHE:HB3	1:B:298:ASN:HB2	2.01	0.43
1:B:335:PHE:HA	5:B:1320:HOH:O	2.18	0.43
1:B:339:GLU:HG2	5:B:1582:HOH:O	2.18	0.43
1:B:65:ALA:O	1:B:67:PRO:HD3	2.18	0.43
1:B:242:PHE:CE2	1:B:244:ARG:CB	3.01	0.43
1:A:206:ASN:OD1	1:A:208:ASN:HB2	2.19	0.43
1:B:19:LEU:HB3	1:B:25:LEU:HD13	2.01	0.43
1:B:70:HIS:CD2	1:B:70:HIS:N	2.86	0.42
1:A:341:VAL:HG13	5:A:1621:HOH:O	2.19	0.42
1:B:114:HIS:O	1:B:115:GLY:O	2.37	0.42
1:A:105:PRO:HB2	1:A:143:THR:CG2	2.49	0.42
1:A:142[A]:VAL:HG21	1:A:155[A]:ARG:HG3	2.00	0.42
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.65	0.42
1:B:341:VAL:HG12	1:B:342:ARG:N	2.32	0.42
1:A:241:GLY:O	1:A:242:PHE:C	2.62	0.42
1:B:157:ILE:HG21	5:B:1701:HOH:O	2.17	0.42
1:B:52:VAL:O	1:B:56:VAL:HG23	2.18	0.42
1:A:177:HIS:CE1	1:A:223:PRO:HD3	2.55	0.42
1:A:320:GLN:HE21	1:A:320:GLN:HB3	1.55	0.42
1:B:144:HIS:HB3	1:B:147:ILE:HG13	2.01	0.42
1:B:317:GLU:O	1:B:319:GLN:N	2.53	0.42
1:A:123:MET:O	1:A:127:GLU:HG3	2.20	0.42
1:A:155[B]:ARG:HH11	1:A:155[B]:ARG:CG	2.32	0.42
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.88	0.42
1:B:42:MET:HA	1:B:43:PRO:HD3	1.86	0.41
1:B:219:LEU:HA	1:B:219:LEU:HD23	1.82	0.41
1:A:10:ARG:HD3	1:A:307:VAL:CG1	2.50	0.41
1:A:60[A]:GLN:HE21	1:A:60[A]:GLN:HB3	1.54	0.41
1:A:93:PHE:CD2	1:A:132:ILE:HD12	2.55	0.41
1:B:51:THR:HB	5:B:1634:HOH:O	2.21	0.41
1:A:21:ASP:CA	1:A:25[A]:LEU:HB2	2.50	0.41
1:A:120:ASP:HA	1:A:123:MET:HG2	2.01	0.41
1:B:319:GLN:CG	1:B:320:GLN:N	2.81	0.41
1:B:340:THR:O	1:B:340:THR:HG22	2.20	0.41
1:B:114:HIS:ND1	5:B:1426:HOH:O	2.29	0.41
1:A:243:GLN:HG2	5:A:1618:HOH:O	2.19	0.41
1:B:52:VAL:HG13	1:B:97:VAL:CG2	2.41	0.41
1:B:179:THR:HA	1:B:234:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LEU:HB3	1:A:25[B]:LEU:HD13	2.01	0.41
1:A:28:VAL:O	1:A:29:VAL:C	2.64	0.41
1:A:110:THR:HG21	1:A:115:GLY:HA3	2.03	0.41
1:B:44:ASN:HB3	1:B:104:TYR:CE1	2.56	0.41
1:B:139:HIS:CD2	1:B:139:HIS:C	2.99	0.41
4:B:411:NCD:C4	4:B:411:NCD:N3	2.78	0.41
1:B:19:LEU:HA	1:B:19:LEU:HD23	1.89	0.41
1:B:52:VAL:CG2	1:B:92:GLY:CA	2.99	0.41
1:B:102:KCX:NZ	1:B:104:TYR:CZ	2.89	0.41
1:A:321:VAL:N	1:A:339:GLU:O	2.43	0.40
1:A:10:ARG:HD3	1:A:307:VAL:HG12	2.02	0.40
1:A:21:ASP:HA	1:A:25[B]:LEU:HB2	2.04	0.40
1:A:162:GLU:CB	1:A:163:PRO:HD3	2.51	0.40
1:A:162:GLU:CB	1:A:163:PRO:CD	2.99	0.40
1:A:319:GLN:O	1:A:340:THR:HA	2.22	0.40
1:B:158:GLU:H	1:B:158:GLU:HG3	1.33	0.40
1:A:70:HIS:CD2	1:A:70:HIS:H	2.39	0.40
1:B:19:LEU:HD13	1:B:29:VAL:HG12	2.02	0.40
1:B:199:THR:HB	1:B:200:PRO:HD2	2.03	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)
5:A:1316:HOH:O	5:A:1687:HOH:O[1_455]	2.19	0.01

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	351/347 (101%)	333 (95%)	16 (5%)	2 (1%)	21 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	337/347 (97%)	309 (92%)	23 (7%)	5 (2%)	8	1
All	All	688/694 (99%)	642 (93%)	39 (6%)	7 (1%)	14	3

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	318	GLU
1	A	177	HIS
1	B	115	GLY
1	B	177	HIS
1	B	91[A]	ARG
1	B	91[B]	ARG
1	A	68	ALA

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	302/295 (102%)	275 (91%)	27 (9%)	9	2
1	B	291/295 (99%)	265 (91%)	26 (9%)	9	2
All	All	593/590 (100%)	540 (91%)	53 (9%)	10	2

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	11[A]	ARG
1	A	11[B]	ARG
1	A	35	ILE
1	A	60[A]	GLN
1	A	60[B]	GLN
1	A	91	ARG
1	A	120	ASP
1	A	123	MET

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Mol	Chain	Res	Type
1	A	125	VAL
1	A	131[A]	LYS
1	A	131[B]	LYS
1	A	155[A]	ARG
1	A	155[B]	ARG
1	A	158	GLU
1	A	162	GLU
1	A	172	LYS
1	A	192	GLU
1	A	224	ILE
1	A	227	ARG
1	A	243	GLN
1	A	289	GLN
1	A	296	SER
1	A	312	ILE
1	A	319	GLN
1	A	341	VAL
1	A	344	SER
1	B	4	SER
1	B	88	GLU
1	B	89	LEU
1	B	91[A]	ARG
1	B	91[B]	ARG
1	B	107	ASN
1	B	113	SER
1	B	123	MET
1	B	131	LYS
1	B	146	ASP
1	B	158	GLU
1	B	159	SER
1	B	165	ARG
1	B	167	ARG
1	B	224	ILE
1	B	229	ILE
1	B	243	GLN
1	B	244	ARG
1	B	286	ASN
1	B	289	GLN
1	B	315	VAL
1	B	318	GLU
1	B	319	GLN
1	B	320	GLN

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Mol	Chain	Res	Type
1	B	340	THR
1	B	344	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	289	GLN
1	A	319	GLN
1	A	320	GLN
1	B	5	GLN
1	B	60	GLN
1	B	107	ASN
1	B	144	HIS
1	B	243	GLN
1	B	257	HIS
1	B	289	GLN
1	B	319	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KCX	B	102	1,2	10,11,12	2.07	1 (10%)	6,12,14	4.04	1 (16%)
1	KCX	A	102	1,2	10,11,12	2.04	1 (10%)	6,12,14	3.80	1 (16%)

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
1	KCX	B	102	1,2	-	1/9/10/12	-
1	KCX	A	102	1,2	-	1/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	KCX	CX-NZ	6.31	1.46	1.35
1	A	102	KCX	CX-NZ	6.18	1.46	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	KCX	CE-NZ-CX	-9.63	105.64	121.98
1	A	102	KCX	CE-NZ-CX	-9.15	106.45	121.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	102	KCX	CG-CD-CE-NZ
1	A	102	KCX	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	102	KCX	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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
3	ORO	A	410	-	11,11,11	3.45	4 (36%)	14,15,15	3.93	4 (28%)
4	NCD	A	950	-	11,11,11	1.42	2 (18%)	13,14,14	1.86	5 (38%)
4	NCD	B	411	2	11,11,11	1.01	0	13,14,14	1.59	3 (23%)

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	ORO	A	410	-	-	2/4/4/4	0/1/1/1
4	NCD	A	950	-	-	2/12/12/12	-
4	NCD	B	411	2	-	3/12/12/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	410	ORO	C2-N1	6.41	1.48	1.37
3	A	410	ORO	C6-N1	6.21	1.51	1.38
3	A	410	ORO	C5-C6	4.87	1.46	1.36
3	A	410	ORO	C5-C4	-4.13	1.34	1.42
4	A	950	NCD	O61-C61	-2.25	1.23	1.30
4	A	950	NCD	C6-C61	2.12	1.58	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	410	ORO	C5-C6-N1	-11.43	107.48	120.87
3	A	410	ORO	C6-N1-C2	-6.81	115.37	122.65
3	A	410	ORO	C7-C6-N1	-4.36	107.52	115.47
4	A	950	NCD	O61-C61-O62	-3.99	115.03	124.08
3	A	410	ORO	C4-N3-C2	-3.12	122.53	125.55
4	B	411	NCD	O2-C2-N3	-2.74	117.67	123.18
4	A	950	NCD	O2-C2-N3	-2.66	117.82	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	411	NCD	O61-C61-O62	-2.54	118.33	124.08
4	A	950	NCD	O61-C61-C6	2.50	121.97	113.51
4	A	950	NCD	O5-C4-C5	2.27	121.07	114.00
4	A	950	NCD	N3-C2-N1	2.21	121.62	116.77
4	B	411	NCD	N3-C2-N1	2.20	121.61	116.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	410	ORO	C5-C6-C7-O71
3	A	410	ORO	C5-C6-C7-O72
4	A	950	NCD	O2-C2-N1-C6
4	A	950	NCD	N3-C2-N1-C6
4	B	411	NCD	O2-C2-N1-C6
4	B	411	NCD	N3-C2-N1-C6
4	B	411	NCD	C61-C6-N1-C2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	950	NCD	5	0
4	B	411	NCD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	342/347 (98%)	0.19	11 (3%)	50 54	13, 24, 50, 78	11 (3%)
1	B	338/347 (97%)	0.63	29 (8%)	16 17	16, 31, 62, 92	3 (0%)
All	All	680/694 (97%)	0.41	40 (5%)	28 31	13, 28, 58, 92	14 (2%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	THR	5.2
1	A	4	SER	3.6
1	B	108	ALA	3.5
1	B	57	ALA	3.4
1	A	108	ALA	3.2
1	B	68	ALA	3.2
1	B	116	VAL	3.2
1	B	328	THR	3.1
1	B	107	ASN	3.1
1	A	68	ALA	3.0
1	A	118	SER	3.0
1	B	113	SER	3.0
1	B	6	VAL	2.9
1	B	125	VAL	2.9
1	B	341	VAL	2.9
1	B	106	ALA	2.8
1	B	4	SER	2.8
1	B	115	GLY	2.6
1	B	119	VAL	2.6
1	B	93	PHE	2.6
1	B	89	LEU	2.6
1	B	190	GLY	2.5
1	B	344	SER	2.5
1	B	7	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	163	PRO	2.4
1	A	94	ASN	2.4
1	B	169	THR	2.4
1	B	340	THR	2.4
1	A	107[A]	ASN	2.3
1	B	170	ALA	2.2
1	A	93	PHE	2.2
1	B	142	VAL	2.1
1	B	339	GLU	2.1
1	B	346	LYS	2.1
1	B	118	SER	2.1
1	A	52	VAL	2.1
1	B	158	GLU	2.1
1	B	163	PRO	2.0
1	A	315	VAL	2.0
1	B	56	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	B	102	12/13	0.92	0.12	20,27,32,52	0
1	KCX	A	102	12/13	0.97	0.06	16,19,27,30	0

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
4	NCD	A	950	12/12	0.74	0.16	37,45,71,77	0
4	NCD	B	411	12/12	0.90	0.12	24,30,40,48	0
3	ORO	A	410	11/11	0.97	0.08	17,21,39,100	0
2	ZN	B	401	1/1	0.98	0.07	35,35,35,35	0
2	ZN	B	400	1/1	0.98	0.05	30,30,30,30	0
2	ZN	A	400	1/1	0.99	0.04	22,22,22,22	0
2	ZN	A	401	1/1	1.00	0.04	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.