



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:19 AM UTC

PDB ID : 1POK / pdb_00001pok
Title : Crystal structure of Isoaspartyl Dipeptidase
Authors : Jozic, D.; Kaiser, J.T.; Huber, R.; Bode, W.; Maskos, K.
Deposited on : 2003-06-15
Resolution : 2.70 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

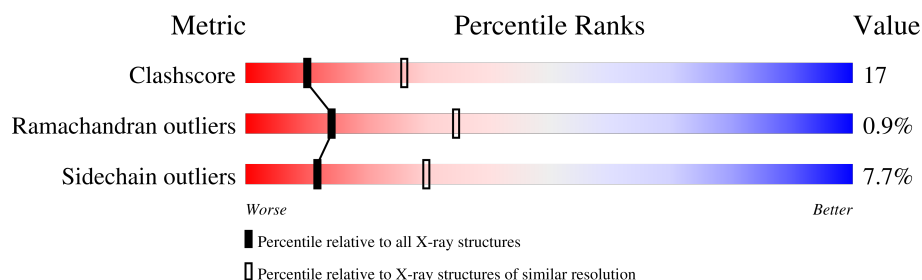
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	390	
1	B	390	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5655 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.

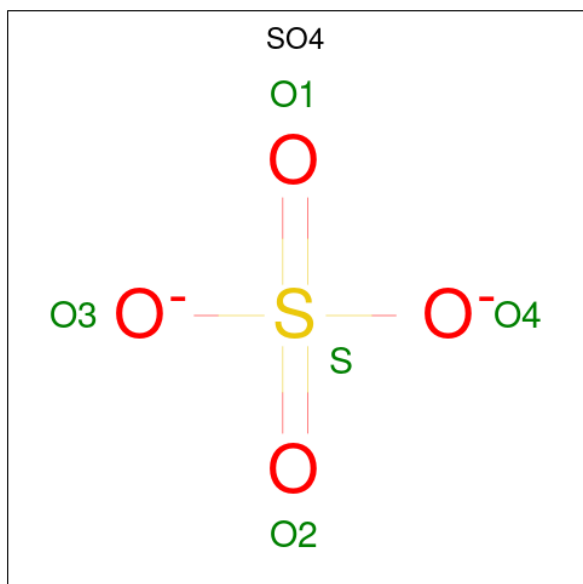
- Molecule 1 is a protein called Isoaspartyl dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	374	Total	C	N	O	S	0	0	0
			2756	1734	473	537	12			
1	A	377	Total	C	N	O	S	0	0	0
			2778	1748	478	540	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	162	KCX	LYS	modified residue	UNP P39377
A	162	KCX	LYS	modified residue	UNP P39377

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	O S	0	0
			5	4 1		

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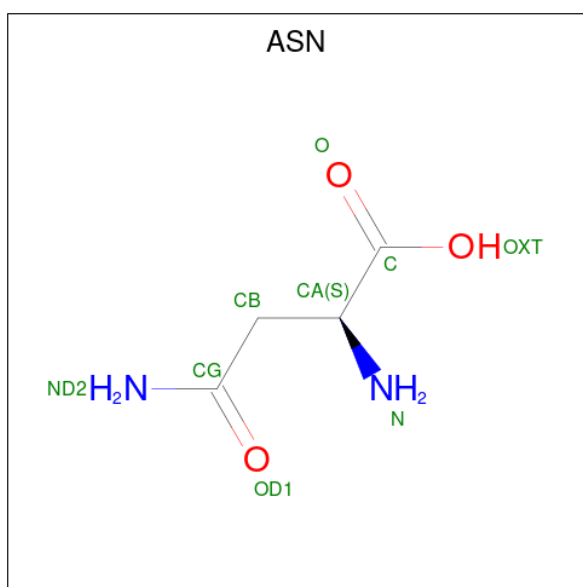
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is ASPARAGINE (CCD ID: ASN) (formula: C₄H₈N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			9	4	2	3		
4	A	1	Total	C	N	O	0	0
			9	4	2	3		

- Molecule 5 is water.

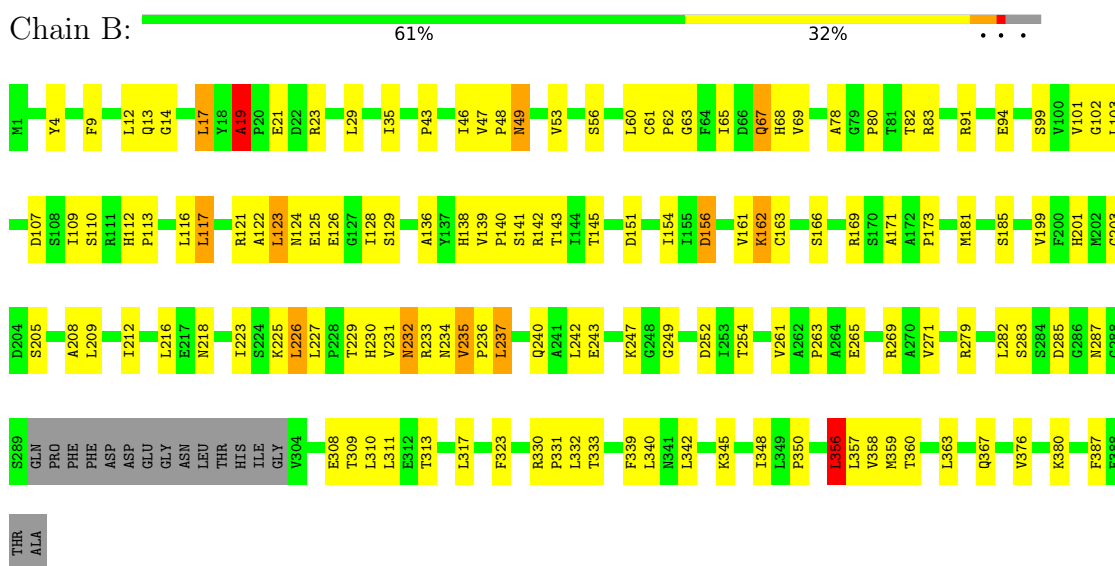
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	42	Total	O	0	0
			42	42		
5	A	47	Total	O	0	0
			47	47		

3 Residue-property plots

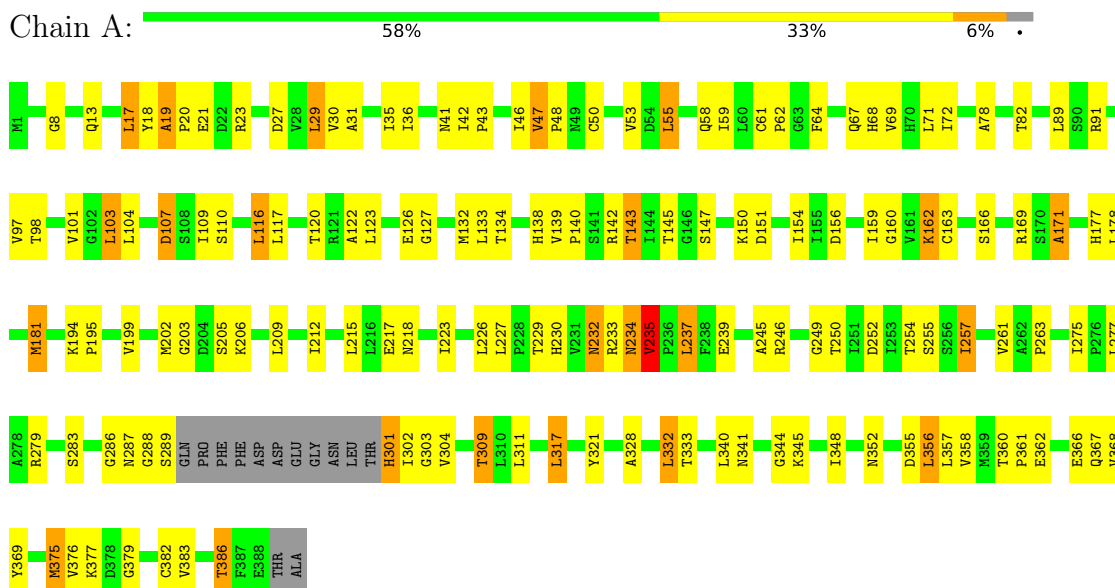
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: Isoaspartyl dipeptidase



- Molecule 1: Isoaspartyl dipeptidase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.47Å 117.47Å 137.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.209 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5655	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, SO4, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/2811	1.06	21/3825 (0.5%)
1	B	0.44	0/2788	1.00	18/3794 (0.5%)
All	All	0.46	0/5599	1.03	39/7619 (0.5%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	TYR	N-CA-C	-9.13	95.53	109.41
1	A	23	ARG	N-CA-C	-7.24	97.49	109.80
1	B	154	ILE	N-CA-C	7.20	122.08	113.22
1	A	379	GLY	N-CA-C	-7.04	105.61	115.32
1	A	154	ILE	N-CA-C	6.99	121.82	113.22
1	A	142	ARG	N-CA-C	-6.77	98.89	109.25
1	B	23	ARG	N-CA-C	-6.60	99.57	109.94
1	B	19	ALA	N-CA-C	6.58	124.36	109.81
1	B	13	GLN	N-CA-C	6.41	120.13	109.95
1	B	138	HIS	N-CA-C	6.38	119.54	109.96
1	A	127	GLY	N-CA-C	6.38	122.07	114.48
1	A	109	ILE	N-CA-C	-6.18	106.89	111.90
1	A	19	ALA	N-CA-C	6.11	123.31	109.81
1	B	141	SER	N-CA-C	6.08	119.28	110.28
1	B	109	ILE	N-CA-C	-6.04	107.05	112.12
1	B	156	ASP	N-CA-C	5.90	119.30	111.75
1	A	171	ALA	N-CA-C	-5.85	105.46	113.30
1	A	97	VAL	N-CA-C	5.65	115.70	108.12
1	B	218	ASN	N-CA-C	5.55	119.92	113.20
1	A	235	VAL	CB-CA-C	-5.52	108.45	113.70
1	A	218	ASN	N-CA-C	5.51	119.00	112.72
1	A	143	THR	N-CA-C	5.46	117.55	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	GLY	N-CA-C	5.36	118.09	111.93
1	B	387	PHE	N-CA-C	5.32	117.69	110.88
1	B	285	ASP	N-CA-C	-5.31	105.44	112.24
1	A	41	ASN	N-CA-C	5.30	117.12	110.91
1	A	386	THR	N-CA-C	5.30	119.23	112.34
1	A	107	ASP	N-CA-C	5.29	116.86	108.67
1	B	171	ALA	N-CA-C	-5.26	106.09	112.88
1	B	67	GLN	N-CA-C	5.19	118.43	112.57
1	B	17	LEU	N-CA-C	5.15	117.16	109.59
1	B	145	THR	CA-C-N	-5.12	117.87	123.30
1	B	145	THR	C-N-CA	-5.12	117.87	123.30
1	A	13	GLN	N-CA-C	5.11	117.58	109.50
1	A	235	VAL	N-CA-C	5.11	119.06	112.67
1	A	47	VAL	CA-C-N	5.11	126.23	119.84
1	A	47	VAL	C-N-CA	5.11	126.23	119.84
1	B	360	THR	N-CA-C	-5.09	104.28	110.13
1	B	356	LEU	N-CA-C	5.01	117.29	109.52

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	2778	0	2800	101	0
1	B	2756	0	2779	91	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	9	0	5	1	0
4	B	9	0	5	2	0
5	A	47	0	0	1	0
5	B	42	0	0	3	0
All	All	5655	0	5589	192	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 17.

All (192) 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:234:ASN:HD22	1:B:236:PRO:HD2	1.35	0.91
1:B:235:VAL:HG13	1:B:236:PRO:HD3	1.53	0.90
1:A:232:ASN:HD22	1:A:232:ASN:H	1.19	0.85
1:B:232:ASN:HD22	1:B:232:ASN:H	1.29	0.78
1:A:78:ALA:HB3	1:A:82:THR:HG21	1.68	0.76
1:A:62:PRO:HG2	1:A:333:THR:HG21	1.68	0.75
1:A:375:MET:HE3	1:A:383:VAL:HG11	1.68	0.75
1:A:159:ILE:HB	1:A:195:PRO:HD2	1.69	0.75
1:B:123:LEU:HG	1:B:128:ILE:HD11	1.68	0.73
1:A:360:THR:HG22	1:A:366:GLU:OE1	1.89	0.72
1:B:63:GLY:HA2	1:B:357:LEU:HG	1.72	0.72
1:B:78:ALA:HB3	1:B:82:THR:HG21	1.71	0.71
1:A:232:ASN:HD22	1:A:232:ASN:N	1.87	0.71
1:A:246:ARG:HG2	1:A:275:ILE:HD11	1.72	0.71
1:A:202:MET:HE2	1:A:209:LEU:HD23	1.73	0.71
1:A:29:LEU:HD13	1:A:36:ILE:HD11	1.74	0.69
1:A:166:SER:HB3	1:A:205:SER:HB3	1.74	0.69
1:B:17:LEU:HD23	1:B:60:LEU:HD23	1.74	0.68
1:B:62:PRO:HG2	1:B:333:THR:HG21	1.75	0.68
1:A:233:ARG:HA	1:A:257:ILE:CD1	2.24	0.67
1:B:61:CYS:HB2	1:B:62:PRO:HD2	1.78	0.66
1:B:229:THR:HG23	1:B:252:ASP:OD1	1.96	0.65
1:A:68:HIS:HD1	1:A:229:THR:HG21	1.62	0.64
1:A:17:LEU:HD23	1:A:18:TYR:N	2.12	0.64
1:A:68:HIS:HA	1:A:103:LEU:HD11	1.80	0.64
1:B:162:KCX:HD2	1:B:163:CYS:N	2.14	0.63
1:A:43:PRO:HG2	1:A:46:ILE:HB	1.80	0.62
1:A:206:LYS:HB3	1:A:206:LYS:NZ	2.14	0.62
1:A:229:THR:HG23	1:A:252:ASP:OD1	2.00	0.61
1:B:35:ILE:O	1:B:350:PRO:HA	2.01	0.60
1:B:227:LEU:HB2	1:B:339:PHE:CZ	2.36	0.60
1:A:138:HIS:HA	1:A:171:ALA:HB2	1.82	0.60
1:A:67:GLN:HA	1:A:101:VAL:HB	1.84	0.59
1:B:199:VAL:HG22	1:B:227:LEU:HD23	1.84	0.59
1:A:17:LEU:HD23	1:A:18:TYR:H	1.66	0.59
1:B:271:VAL:HG21	1:B:323:PHE:CE1	2.38	0.59
1:A:229:THR:HG22	1:A:230:HIS:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ASN:H	1:B:232:ASN:ND2	1.98	0.58
1:B:4:TYR:HB2	1:B:49:ASN:HD22	1.67	0.58
1:B:282:LEU:HD23	1:B:332:LEU:HD13	1.84	0.58
1:B:12:LEU:HD11	1:B:356:LEU:HD13	1.86	0.57
1:A:227:LEU:HD11	1:A:252:ASP:HB2	1.86	0.57
1:A:233:ARG:HA	1:A:257:ILE:HD11	1.85	0.57
1:A:288:GLY:O	1:A:289:SER:HB2	2.02	0.57
1:B:234:ASN:ND2	1:B:237:LEU:H	2.03	0.57
1:A:47:VAL:HG23	1:A:50:CYS:HB2	1.87	0.56
1:A:358:VAL:HB	1:A:367:GLN:HB2	1.86	0.56
1:B:229:THR:HG22	1:B:230:HIS:H	1.70	0.56
1:B:35:ILE:HD13	1:B:348:ILE:HG23	1.88	0.56
1:B:249:GLY:O	1:B:279:ARG:HD2	2.05	0.56
1:A:317:LEU:HD23	1:A:328:ALA:HA	1.88	0.56
1:B:212:ILE:O	1:B:216:LEU:HD13	2.05	0.56
1:B:143:THR:HB	1:B:151:ASP:OD1	2.06	0.55
1:B:12:LEU:HD23	1:B:53:VAL:CG1	2.37	0.55
1:A:61:CYS:HB2	1:A:62:PRO:HD2	1.89	0.55
1:B:310:LEU:HD22	1:B:332:LEU:HD11	1.89	0.55
1:A:169:ARG:HH22	4:A:400:ASN:HB2	1.70	0.55
1:A:145:THR:OG1	1:A:150:LYS:HB3	2.07	0.54
1:B:65:ILE:HG12	1:B:99:SER:HB2	1.89	0.54
1:A:139:VAL:HA	1:A:140:PRO:C	2.30	0.54
1:A:230:HIS:CD2	1:A:254:THR:HG21	2.43	0.54
1:A:223:ILE:HA	1:A:226:LEU:HD23	1.89	0.54
1:A:358:VAL:CG2	1:A:367:GLN:HB2	2.37	0.54
1:B:229:THR:HG22	1:B:230:HIS:N	2.23	0.53
1:A:133:LEU:HD11	1:A:199:VAL:HG21	1.89	0.53
1:A:232:ASN:H	1:A:232:ASN:ND2	1.94	0.53
1:B:80:PRO:O	1:B:83:ARG:HG3	2.08	0.53
1:B:227:LEU:HD11	1:B:252:ASP:HB2	1.90	0.53
1:B:107:ASP:OD1	1:B:110:SER:OG	2.27	0.53
1:B:166:SER:HB3	1:B:205:SER:HB3	1.90	0.52
1:B:12:LEU:HD23	1:B:53:VAL:HG11	1.90	0.52
1:A:68:HIS:ND1	1:A:229:THR:HG21	2.25	0.52
1:B:330:ARG:HB2	1:B:331:PRO:HD3	1.90	0.52
1:B:14:GLY:O	1:B:56:SER:HA	2.09	0.52
1:A:72:ILE:HD11	1:A:104:LEU:HD21	1.92	0.52
1:A:345:LYS:NZ	1:A:355:ASP:OD2	2.43	0.52
1:B:43:PRO:HB2	1:B:46:ILE:HB	1.90	0.52
1:B:122:ALA:O	1:B:126:GLU:HG3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ILE:HD13	1:A:356:LEU:HD23	1.92	0.51
1:B:68:HIS:HB2	1:B:283:SER:HB2	1.93	0.51
1:A:107:ASP:OD1	1:A:110:SER:OG	2.28	0.51
1:A:250:THR:HG23	1:A:279:ARG:HA	1.92	0.51
1:B:208:ALA:HB1	1:B:237:LEU:HD23	1.93	0.50
1:B:367:GLN:HA	1:B:376:VAL:O	2.12	0.50
1:A:301:HIS:O	1:A:302:ILE:HD13	2.10	0.50
1:A:55:LEU:O	1:A:58:GLN:HB2	2.10	0.50
1:B:142:ARG:HG2	1:B:142:ARG:HH11	1.76	0.50
1:A:311:LEU:HD23	1:A:311:LEU:O	2.11	0.50
1:A:209:LEU:HD22	1:A:212:ILE:HD12	1.94	0.49
1:A:226:LEU:HD22	1:A:226:LEU:N	2.27	0.49
1:A:68:HIS:HD2	1:A:103:LEU:HD21	1.77	0.49
1:B:19:ALA:HA	1:B:348:ILE:HD12	1.94	0.49
1:B:124:ASN:HA	1:B:128:ILE:O	2.13	0.49
1:B:282:LEU:HB3	1:B:332:LEU:HD13	1.95	0.49
1:B:223:ILE:HA	1:B:226:LEU:CD2	2.43	0.49
1:B:9:PHE:HB2	1:B:49:ASN:O	2.12	0.49
1:A:255:SER:HB2	1:A:309:THR:HB	1.94	0.49
1:A:230:HIS:HD2	1:A:254:THR:HG21	1.78	0.48
1:A:145:THR:HB	1:A:150:LYS:HD3	1.96	0.48
1:A:344:GLY:HA2	1:A:352:ASN:OD1	2.14	0.48
1:A:255:SER:HA	1:A:263:PRO:HG3	1.95	0.48
1:A:234:ASN:ND2	1:A:237:LEU:H	2.11	0.48
1:A:195:PRO:HG3	1:A:340:LEU:O	2.13	0.47
1:A:232:ASN:HB2	1:A:261:VAL:HB	1.94	0.47
1:B:313:THR:O	1:B:317:LEU:HB2	2.15	0.47
1:B:12:LEU:CD1	1:B:356:LEU:HD13	2.44	0.47
1:B:161:VAL:HG12	1:B:185:SER:HB2	1.97	0.47
1:B:234:ASN:HD22	1:B:236:PRO:CD	2.17	0.47
1:B:282:LEU:HB3	1:B:332:LEU:CD1	2.44	0.47
1:A:35:ILE:HD13	1:A:348:ILE:HG23	1.96	0.47
1:A:178:LEU:HD12	1:A:181:MET:CE	2.45	0.47
1:B:231:VAL:HA	1:B:237:LEU:CD1	2.45	0.47
1:B:203:GLY:O	1:B:233:ARG:HD3	2.14	0.46
1:A:116:LEU:HD13	1:A:132:MET:HB2	1.97	0.46
1:A:203:GLY:O	1:A:233:ARG:HD3	2.16	0.46
1:B:139:VAL:HA	1:B:140:PRO:C	2.40	0.46
1:B:232:ASN:HD21	1:B:254:THR:H	1.62	0.46
1:A:367:GLN:HA	1:A:376:VAL:O	2.14	0.46
1:B:83:ARG:NH1	5:B:630:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:GLU:OE1	1:B:247:LYS:HE3	2.15	0.46
1:A:68:HIS:CD2	1:A:103:LEU:HD21	2.50	0.46
1:B:223:ILE:HA	1:B:226:LEU:HD23	1.98	0.46
1:A:64:PHE:CE1	1:A:332:LEU:HD23	2.51	0.46
1:B:225:LYS:HE3	5:B:611:HOH:O	2.14	0.46
1:B:308:GLU:HG2	1:B:309:THR:N	2.29	0.46
1:A:27:ASP:HB2	1:A:42:ILE:HG13	1.98	0.46
1:A:134:THR:HG22	1:A:160:GLY:O	2.16	0.46
1:A:355:ASP:HA	1:A:369:TYR:O	2.15	0.46
1:A:245:ALA:HA	1:A:249:GLY:O	2.16	0.45
1:A:250:THR:HG23	1:A:279:ARG:C	2.42	0.45
1:A:301:HIS:HD1	1:A:301:HIS:N	2.14	0.45
1:B:99:SER:OG	1:B:345:LYS:HD3	2.16	0.45
1:A:143:THR:HB	1:A:151:ASP:OD1	2.17	0.45
1:B:46:ILE:HG23	1:B:47:VAL:HG22	1.98	0.45
1:B:123:LEU:HD12	1:B:123:LEU:HA	1.79	0.45
1:A:255:SER:HA	1:A:263:PRO:CG	2.46	0.45
1:B:263:PRO:HD2	5:B:619:HOH:O	2.17	0.45
1:A:18:TYR:C	1:A:20:PRO:HA	2.42	0.44
1:A:162:KCX:HG2	1:A:163:CYS:N	2.31	0.44
1:A:202:MET:HB3	1:A:237:LEU:HD11	2.00	0.44
1:A:206:LYS:HB3	1:A:206:LYS:HZ2	1.79	0.44
1:B:201:HIS:HE1	4:B:401:ASN:N	2.16	0.44
1:A:215:LEU:C	1:A:215:LEU:HD23	2.42	0.44
1:B:232:ASN:HB2	1:B:261:VAL:HB	1.99	0.44
1:A:340:LEU:O	1:A:341:ASN:C	2.60	0.44
1:B:17:LEU:HD11	1:B:19:ALA:HB2	1.99	0.44
1:B:208:ALA:HB3	1:B:240:GLN:OE1	2.18	0.44
1:B:340:LEU:HB2	1:B:342:LEU:HG	1.99	0.43
1:B:139:VAL:HB	1:B:173:PRO:HB3	1.98	0.43
1:B:162:KCX:OQ1	1:B:201:HIS:HB2	2.19	0.43
1:B:169:ARG:NH2	4:B:401:ASN:HA	2.33	0.43
1:A:156:ASP:O	1:A:194:LYS:HE2	2.18	0.43
1:B:358:VAL:HB	1:B:367:GLN:HB2	2.00	0.43
1:A:377:LYS:HB2	1:A:382:CYS:SG	2.58	0.43
1:A:69:VAL:HG12	1:A:71:LEU:HD12	2.00	0.43
1:A:229:THR:CG2	1:A:230:HIS:N	2.82	0.43
1:B:94:GLU:OE1	1:B:380:LYS:HA	2.19	0.43
1:A:30:VAL:HG12	1:A:31:ALA:N	2.33	0.43
1:B:19:ALA:CB	1:B:348:ILE:HB	2.49	0.43
1:B:117:LEU:HD22	1:B:121:ARG:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:O	1:A:239:GLU:HG2	2.19	0.42
1:B:234:ASN:HD21	1:B:237:LEU:H	1.66	0.42
1:B:209:LEU:HD22	1:B:212:ILE:HD12	2.01	0.42
1:A:358:VAL:CB	1:A:367:GLN:HB2	2.49	0.42
1:A:59:ILE:CD1	1:A:361:PRO:HA	2.48	0.42
1:A:147:SER:OG	1:A:150:LYS:HB2	2.20	0.42
1:A:301:HIS:N	1:A:301:HIS:ND1	2.66	0.42
1:B:163:CYS:SG	1:B:181:MET:HE1	2.60	0.41
1:B:112:HIS:HA	1:B:113:PRO:HD3	1.96	0.41
1:A:72:ILE:HD11	1:A:104:LEU:CD2	2.49	0.41
1:A:177:HIS:O	1:A:181:MET:HB2	2.21	0.41
1:A:357:LEU:HD23	1:A:368:VAL:HG13	2.01	0.41
1:A:226:LEU:HD22	1:A:226:LEU:H	1.86	0.41
1:B:65:ILE:HA	1:B:99:SER:O	2.21	0.41
1:B:136:ALA:O	1:B:163:CYS:HA	2.21	0.41
1:B:271:VAL:HG21	1:B:323:PHE:HE1	1.82	0.41
1:B:359:MET:HE2	1:B:363:LEU:C	2.44	0.41
1:A:229:THR:HG22	1:A:230:HIS:H	1.84	0.41
1:B:67:GLN:HA	1:B:101:VAL:HB	2.02	0.41
1:A:122:ALA:O	1:A:126:GLU:HG3	2.20	0.41
1:B:69:VAL:O	1:B:102:GLY:HA2	2.21	0.41
1:B:265:GLU:HG3	1:B:269:ARG:HD2	2.02	0.41
1:A:8:GLY:HA2	5:A:642:HOH:O	2.21	0.41
1:A:166:SER:O	1:A:203:GLY:HA3	2.21	0.41
1:A:254:THR:HA	1:A:283:SER:O	2.20	0.41
1:B:21:GLU:H	1:B:21:GLU:CD	2.29	0.41
1:A:229:THR:HG22	1:A:230:HIS:CD2	2.56	0.40
1:B:129:SER:CB	1:B:345:LYS:HE3	2.51	0.40
1:A:68:HIS:CD2	1:A:103:LEU:HD11	2.56	0.40
1:A:234:ASN:ND2	1:A:234:ASN:C	2.79	0.40
1:B:121:ARG:O	1:B:125:GLU:HG3	2.21	0.40
1:A:230:HIS:O	1:A:233:ARG:HG2	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	372/390 (95%)	342 (92%)	26 (7%)	4 (1%)	11	29
1	B	369/390 (95%)	337 (91%)	29 (8%)	3 (1%)	16	37
All	All	741/780 (95%)	679 (92%)	55 (7%)	7 (1%)	14	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	48	PRO
1	A	48	PRO
1	A	303	GLY
1	B	49	ASN
1	A	309	THR
1	A	19	ALA
1	B	19	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	299/312 (96%)	269 (90%)	30 (10%)	7	19
1	B	297/312 (95%)	282 (95%)	15 (5%)	21	48
All	All	596/624 (96%)	551 (92%)	45 (8%)	12	30

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	29	LEU
1	B	91	ARG
1	B	103	LEU
1	B	116	LEU
1	B	117	LEU

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Mol	Chain	Res	Type
1	B	123	LEU
1	B	156	ASP
1	B	226	LEU
1	B	232	ASN
1	B	235	VAL
1	B	237	LEU
1	B	242	LEU
1	B	287	ASN
1	B	311	LEU
1	B	356	LEU
1	A	17	LEU
1	A	21	GLU
1	A	29	LEU
1	A	53	VAL
1	A	55	LEU
1	A	89	LEU
1	A	91	ARG
1	A	98	THR
1	A	103	LEU
1	A	116	LEU
1	A	117	LEU
1	A	120	THR
1	A	123	LEU
1	A	181	MET
1	A	217	GLU
1	A	232	ASN
1	A	234	ASN
1	A	235	VAL
1	A	237	LEU
1	A	257	ILE
1	A	277	LEU
1	A	287	ASN
1	A	301	HIS
1	A	304	VAL
1	A	317	LEU
1	A	332	LEU
1	A	356	LEU
1	A	362	GLU
1	A	375	MET
1	A	386	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	32	ASN
1	B	41	ASN
1	B	49	ASN
1	B	67	GLN
1	B	180	ASN
1	B	201	HIS
1	B	218	ASN
1	B	232	ASN
1	B	234	ASN
1	B	367	GLN
1	A	32	ASN
1	A	49	ASN
1	A	67	GLN
1	A	68	HIS
1	A	232	ASN
1	A	234	ASN
1	A	287	ASN
1	A	315	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	162	1,3	10,11,12	0.91	1 (10%)	6,12,14	1.31	1 (16%)
1	KCX	A	162	1,3	10,11,12	0.94	1 (10%)	6,12,14	1.19	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	162	1,3	-	2/9/10/12	-
1	KCX	A	162	1,3	-	0/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	KCX	OQ1-CX	2.46	1.26	1.21
1	B	162	KCX	OQ1-CX	2.28	1.25	1.21

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	KCX	OQ1-CX-NZ	-2.78	120.70	124.92
1	A	162	KCX	OQ1-CX-NZ	-2.26	121.49	124.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	162	KCX	CA-CB-CG-CD
1	B	162	KCX	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	162	KCX	2	0
1	A	162	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ASN	A	400	-	7,8,8	0.82	0	6,10,10	0.24	0
2	SO4	A	391	-	4,4,4	0.35	0	6,6,6	0.09	0
4	ASN	B	401	-	7,8,8	0.77	0	6,10,10	0.31	0
2	SO4	B	391	-	4,4,4	0.36	0	6,6,6	0.07	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
4	ASN	A	400	-	-	4/8/8/8	-
4	ASN	B	401	-	-	2/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	400	ASN	C-CA-CB-CG
4	A	400	ASN	CA-CB-CG-OD1
4	A	400	ASN	CA-CB-CG-ND2
4	A	400	ASN	N-CA-CB-CG
4	B	401	ASN	O-C-CA-CB
4	B	401	ASN	OXT-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	400	ASN	1	0
4	B	401	ASN	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.