



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 10:25 pm BST

PDB ID : 1POK  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

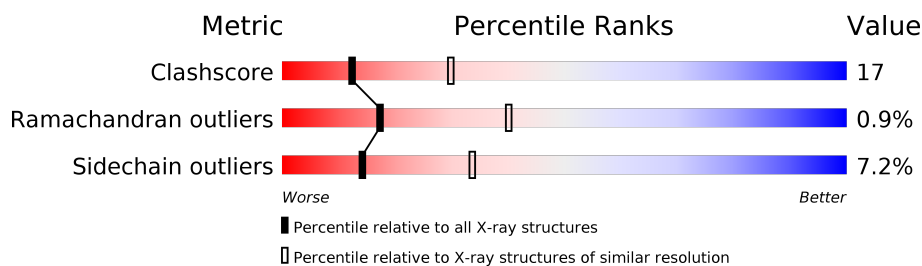
# 1 Overall quality at a glance

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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
			Total	C	N	O	S			
1	B	374	2756	1734	473	537	12	0	0	0
1	A	377	2778	1748	478	540	12	0	0	0

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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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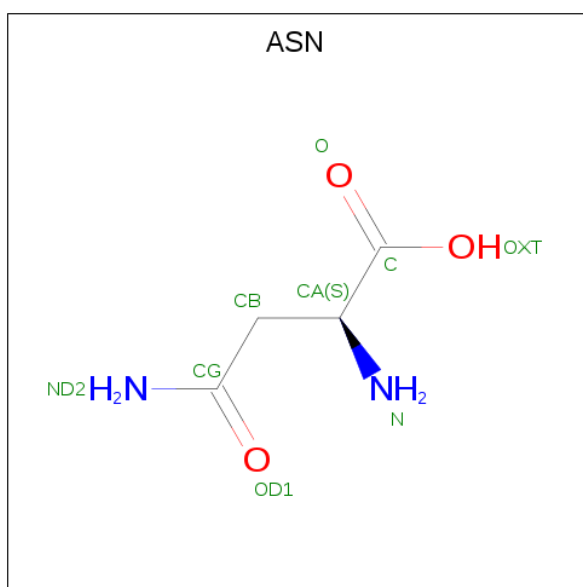
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ZINC ION (three-letter code: 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 (three-letter code: ASN) (formula: C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O<sub>3</sub>).



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.

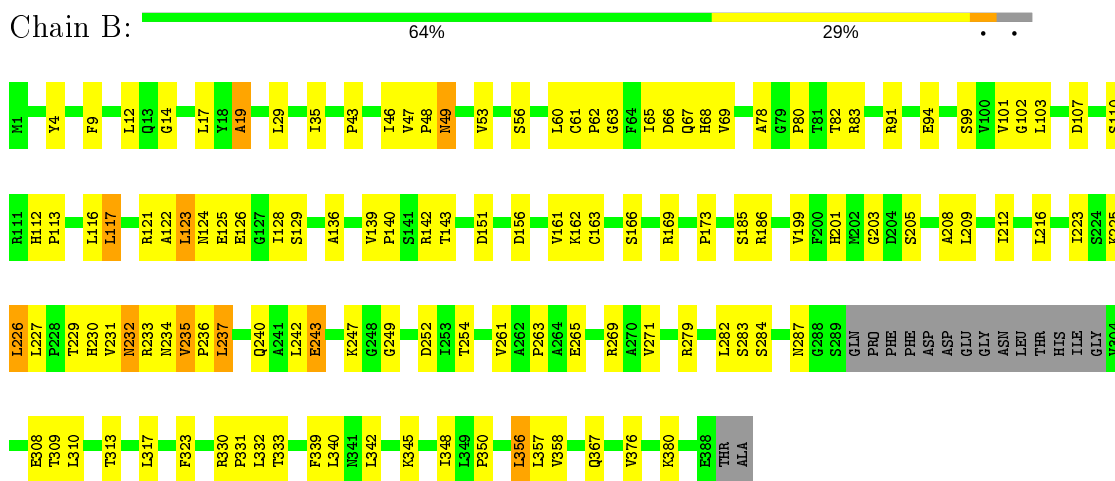
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	42	Total	O	0	0
			42	42		
5	A	47	Total	O	0	0
			47	47		

### 3 Residue-property plots

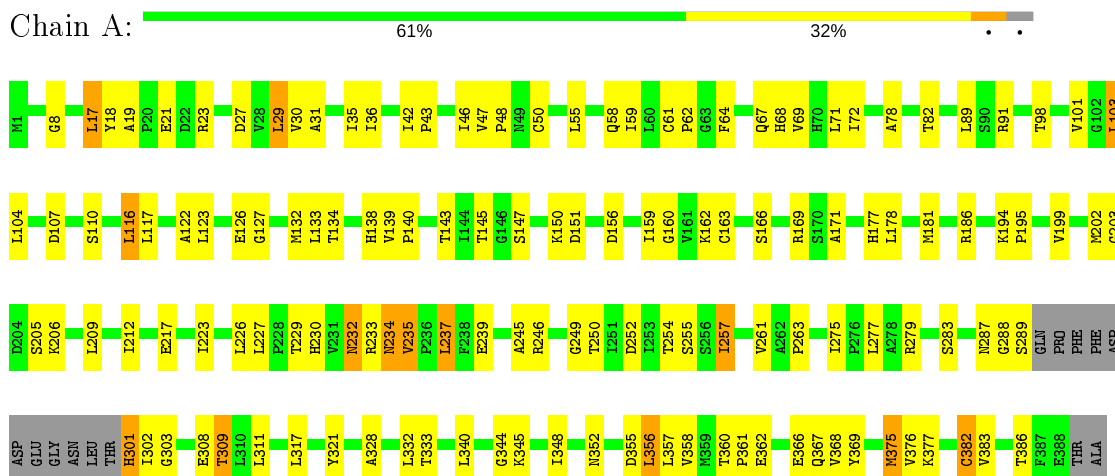
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	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.	Xtrriage
Total number of atoms	5655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, 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	0.37	0/2811	0.71	2/3825 (0.1%)
1	B	0.36	0/2788	0.67	0/3794
All	All	0.36	0/5599	0.69	2/7619 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	TYR	N-CA-C	-5.73	95.53	111.00
1	A	23	ARG	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	99	0
1	B	2756	0	2779	89	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	188	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 (188) 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:H	1:A:232:ASN:HD22	1.19	0.85
1:B:232:ASN:H	1:B:232:ASN:HD22	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: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:A:232:ASN:N	1:A:232:ASN:HD22	1.87	0.71
1:B:78:ALA:HB3	1:B:82:THR:HG21	1.71	0.71
1:A:246:ARG:HG2	1:A:275:ILE:HD11	1.72	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: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:NZ	1:A:206:LYS:HB3	2.14	0.62
1:A:232:ASN:ND2	1:A:232:ASN:H	1.94	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLN:HA	1:A:101:VAL:HB	1.84	0.59
1:A:288:GLY:O	1:A:289:SER:HB2	2.02	0.59
1:A:17:LEU:HD23	1:A:18:TYR:H	1.66	0.59
1:B:199:VAL:HG22	1:B:227:LEU:HD23	1.84	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
1:B:232:ASN:H	1:B:232:ASN:ND2	1.98	0.58
1:B:282:LEU:HD23	1:B:332:LEU:HD13	1.84	0.58
1:B:4:TYR:HB2	1:B:49:ASN:HD22	1.67	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:B:234:ASN:ND2	1:B:237:LEU:H	2.03	0.57
1:A:358:VAL:HB	1:A:367:GLN:HB2	1.86	0.56
1:A:47:VAL:HG23	1:A:50:CYS:HB2	1.87	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:A:317:LEU:HD23	1:A:328:ALA:HA	1.88	0.56
1:B:249:GLY:O	1:B:279:ARG:HD2	2.05	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: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: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: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:A:72:ILE:HD11	1:A:104:LEU:HD21	1.92	0.52
1:B:14:GLY:O	1:B:56:SER:HA	2.09	0.52
1:B:43:PRO:HB2	1:B:46:ILE:HB	1.90	0.52

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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:122:ALA:O	1:B:126:GLU:HG3	2.09	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:A:301:HIS:O	1:A:302:ILE:HD13	2.10	0.50
1:B:367:GLN:HA	1:B:376:VAL:O	2.12	0.50
1:A:55:LEU:O	1:A:58:GLN:HB2	2.10	0.50
1:B:142:ARG:HH11	1:B:142:ARG:HG2	1.76	0.50
1:A:139:VAL:HA	1:A:140:PRO:C	2.30	0.50
1:A:311:LEU:O	1:A:311:LEU:HD23	2.11	0.50
1:A:209:LEU:HD22	1:A:212:ILE:HD12	1.94	0.49
1:A:226:LEU:N	1:A:226:LEU:HD22	2.27	0.49
1:A:375:MET:HE3	1:A:383:VAL:HG11	1.95	0.49
1:A:68:HIS:HD2	1:A:103:LEU:HD21	1.77	0.49
1:B:124:ASN:HA	1:B:128:ILE:O	2.13	0.49
1:B:19:ALA:HA	1:B:348:ILE:HD12	1.94	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:A:255:SER:HB2	1:A:309:THR:HB	1.94	0.49
1:B:9:PHE:HB2	1:B:49:ASN:O	2.12	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:308:GLU:HG2	1:B:309:THR:N	2.29	0.47
1:B:313:THR:O	1:B:317:LEU:HB2	2.15	0.47
1:A:35:ILE:HD13	1:A:348:ILE:HG23	1.96	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:178:LEU:HD12	1:A:181:MET:CE	2.45	0.47
1:B:161:VAL:HG12	1:B:185:SER:HB2	1.97	0.47
1:B:12:LEU:CD1	1:B:356:LEU:HD13	2.44	0.47
1:B:231:VAL:HA	1:B:237:LEU:CD1	2.45	0.47
1:A:116:LEU:HD13	1:A:132:MET:HB2	1.97	0.46
1:B:203:GLY:O	1:B:233:ARG:HD3	2.14	0.46
1:A:203:GLY:O	1:A:233:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLN:HA	1:A:376:VAL:O	2.14	0.46
1:B:232:ASN:HD21	1:B:254:THR:H	1.62	0.46
1:A:68:HIS:CD2	1:A:103:LEU:HD21	2.50	0.46
1:B:107:ASP:OD1	1:B:110:SER:OG	2.27	0.46
1:B:243:GLU:OE1	1:B:247:LYS:HE3	2.15	0.46
1:B:83:ARG:NH1	5:B:630:HOH:O	2.48	0.46
1:A:64:PHE:CE1	1:A:332:LEU:HD23	2.51	0.46
1:B:223:ILE:HA	1:B:226:LEU:HD23	1.98	0.46
1:B:225:LYS:HE3	5:B:611:HOH:O	2.14	0.46
1:A:178:LEU:HD12	1:A:181:MET:HE3	1.97	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:301:HIS:HD1	1:A:301:HIS:N	2.14	0.45
1:A:143:THR:HB	1:A:151:ASP:OD1	2.17	0.45
1:B:99:SER:OG	1:B:345:LYS:HD3	2.16	0.45
1:B:123:LEU:HA	1:B:123:LEU:HD12	1.79	0.45
1:B:46:ILE:HG23	1:B:47:VAL:HG22	1.98	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: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:HZ2	1:A:206:LYS:HB3	1.79	0.44
1:B:201:HIS:HE1	4:B:401:ASN:N	2.16	0.44
1:B:232:ASN:HB2	1:B:261:VAL:HB	1.99	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:A:156:ASP:O	1:A:194:LYS:HE2	2.18	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:377:LYS:HB2	1:A:382:CYS:SG	2.58	0.43
1:B:358:VAL:HB	1:B:367:GLN:HB2	2.00	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:A:30:VAL:HG12	1:A:31:ALA:N	2.33	0.43
1:B:94:GLU:OE1	1:B:380:LYS:HA	2.19	0.43
1:B:117:LEU:HD22	1:B:121:ARG:HD2	2.01	0.43
1:B:19:ALA:CB	1:B:348:ILE:HB	2.49	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:139:VAL:HA	1:B:140:PRO:C	2.40	0.41
1:B:66:ASP:OD2	1:B:284:SER:OG	2.36	0.41
1:A:72:ILE:HD11	1:A:104:LEU:CD2	2.49	0.41
1:B:112:HIS:HA	1:B:113:PRO:HD3	1.96	0.41
1:A:68:HIS:HE2	1:A:162:KCX:CX	2.32	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:H	1:A:226:LEU:HD22	1.86	0.41
1:A:229:THR:HG22	1:A:230:HIS:H	1.84	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:65:ILE:HA	1:B:99:SER:O	2.21	0.41
1:A:122:ALA:O	1:A:126:GLU:HG3	2.20	0.41
1:B:67:GLN:HA	1:B:101:VAL:HB	2.02	0.41
1:A:166:SER:O	1:A:203:GLY:HA3	2.21	0.41
1:B:265:GLU:HG3	1:B:269:ARG:HD2	2.02	0.41
1:A:254:THR:HA	1:A:283:SER:O	2.20	0.41
1:A:8:GLY:HA2	5:A:642:HOH:O	2.21	0.41
1:B:69:VAL:O	1:B:102:GLY:HA2	2.21	0.41
1:A:127:GLY:HA3	1:A:375:MET:HE1	2.03	0.41
1:A:229:THR:HG22	1:A:230:HIS:CD2	2.56	0.40
1:A:250:THR:HG23	1:A:279:ARG:C	2.42	0.40
1:A:68:HIS:CD2	1:A:103:LEU:HD11	2.56	0.40
1:A:375:MET:CE	1:A:383:VAL:HG11	2.51	0.40
1:B:129:SER:CB	1:B:345:LYS:HE3	2.51	0.40
1:A:230:HIS:O	1:A:233:ARG:HG2	2.22	0.40
1:A:345:LYS:NZ	1:A:355:ASP:OD2	2.43	0.40
1:B:121:ARG:O	1:B:125:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/390 (95%)	342 (92%)	26 (7%)	4 (1%)	14	34
1	B	369/390 (95%)	337 (91%)	29 (8%)	3 (1%)	19	43
All	All	741/780 (95%)	679 (92%)	55 (7%)	7 (1%)	17	40

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/312 (96%)	273 (91%)	26 (9%)	10	23
1	B	297/312 (95%)	281 (95%)	16 (5%)	22	47
All	All	596/624 (96%)	554 (93%)	42 (7%)	14	35

All (42) 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
1	B	123	LEU
1	B	156	ASP
1	B	186	ARG
1	B	226	LEU
1	B	232	ASN
1	B	235	VAL
1	B	237	LEU
1	B	242	LEU
1	B	243	GLU
1	B	287	ASN
1	B	356	LEU
1	A	17	LEU
1	A	21	GLU
1	A	29	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	123	LEU
1	A	186	ARG
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	308	GLU
1	A	356	LEU
1	A	362	GLU
1	A	375	MET
1	A	382	CYS
1	A	386	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	32	ASN
1	B	49	ASN
1	B	67	GLN
1	B	201	HIS
1	B	232	ASN
1	B	234	ASN
1	B	315	GLN
1	A	32	ASN
1	A	49	ASN
1	A	67	GLN
1	A	232	ASN
1	A	234	ASN
1	A	315	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	A	162	1,3	7,11,12	0.48	0	4,12,14	0.77	0
1	KCX	B	162	1,3	7,11,12	0.50	0	4,12,14	0.66	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
1	KCX	A	162	1,3	-	0/7/10/12	-
1	KCX	B	162	1,3	-	2/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

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 4 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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
2	SO4	A	391	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	B	391	-	4,4,4	0.25	0	6,6,6	0.12	0



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.

No monomer is involved in short contacts.

## 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.