



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:51 PM UTC

PDB ID : 1ONX / pdb_00001onx
Title : Crystal structure of isoaspartyl dipeptidase from escherichia coli complexed with aspartate
Authors : Thoden, J.B.; Marti-Arbona, R.; Raushel, F.M.; Holden, H.M.
Deposited on : 2003-03-02
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

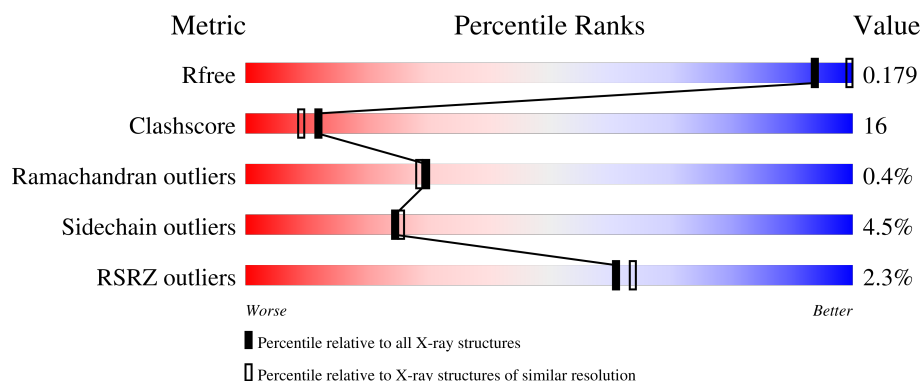
1 Overall quality at a glance

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	390	2% 58% 37% • •
1	B	390	3% 70% 27% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6053 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.

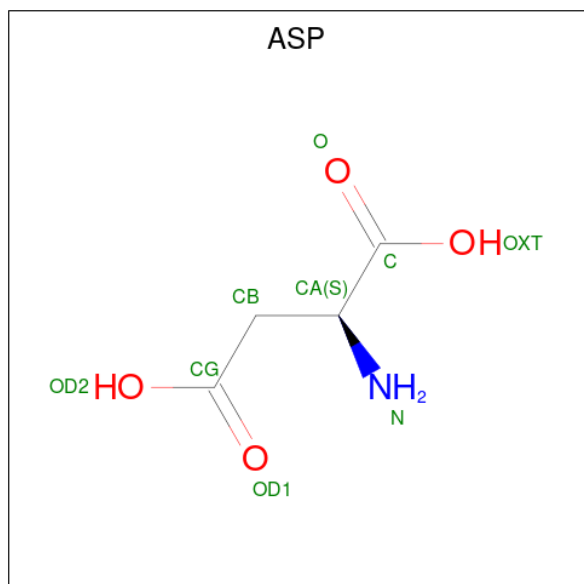
- Molecule 1 is a protein called Isoaspartyl dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	1	0
			2887	1817	495	563	12			
1	B	389	Total	C	N	O	S	0	1	0
			2887	1817	495	563	12			

- 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 ASPARTIC ACID (CCD ID: ASP) (formula: C₄H₇NO₄).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		
4	B	128	Total	O	0	0
			128	128		

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.10Å 119.10Å 138.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.10) 94.3 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.05Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.177 , 0.246 0.178 , 0.179	Depositor DCC
R_{free} test set	5836 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 103.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6053	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 4.00% 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: ZN, 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	1.15	0/2928	1.65	28/3984 (0.7%)
1	B	1.20	1/2928 (0.0%)	1.64	25/3984 (0.6%)
All	All	1.18	1/5856 (0.0%)	1.65	53/7968 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	LEU	N-CA	-5.26	1.39	1.46

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	PRO	CB-CA-C	-9.40	99.19	111.23
1	A	287	ASN	CA-CB-CG	-7.88	104.72	112.60
1	B	41	ASN	N-CA-C	7.58	119.78	110.91
1	B	13	GLN	N-CA-C	7.49	121.13	109.07
1	A	319	LYS	N-CA-C	7.25	118.83	111.07
1	B	70	HIS	CA-CB-CG	-7.17	106.64	113.80
1	A	304	VAL	N-CA-C	7.13	118.32	107.77
1	A	154	ILE	CA-C-N	-7.13	113.59	122.93
1	A	154	ILE	C-N-CA	-7.13	113.59	122.93
1	B	387	PHE	CA-CB-CG	-6.92	106.88	113.80
1	A	19	ALA	N-CA-C	6.91	125.07	109.81
1	B	177	HIS	CA-CB-CG	-6.87	106.93	113.80
1	A	301	HIS	N-CA-CB	-6.80	99.44	111.08
1	A	284	SER	N-CA-C	6.74	119.62	111.40
1	B	19	ALA	N-CA-C	6.67	124.55	109.81
1	A	13	GLN	N-CA-C	6.61	119.71	109.07
1	A	320	ASP	CB-CA-C	-6.59	99.03	110.17
1	B	79	GLY	CA-C-N	6.37	126.85	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	GLY	C-N-CA	6.37	126.85	119.47
1	A	382	CYS	N-CA-C	-6.28	105.65	113.38
1	A	320	ASP	CA-C-N	-6.24	112.43	121.98
1	A	320	ASP	C-N-CA	-6.24	112.43	121.98
1	A	79	GLY	CA-C-N	6.09	125.77	119.56
1	A	79	GLY	C-N-CA	6.09	125.77	119.56
1	B	274	GLY	CA-C-N	-6.04	117.48	123.04
1	B	274	GLY	C-N-CA	-6.04	117.48	123.04
1	A	101	VAL	N-CA-CB	5.99	119.45	111.90
1	A	35	ILE	CA-C-N	-5.85	113.25	121.55
1	A	35	ILE	C-N-CA	-5.85	113.25	121.55
1	B	156	ASP	N-CA-C	5.84	118.11	111.11
1	B	47	VAL	CA-C-N	5.81	125.77	119.78
1	B	47	VAL	C-N-CA	5.81	125.77	119.78
1	B	154	ILE	N-CA-C	5.77	121.87	113.39
1	A	294	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	58	GLN	N-CA-C	5.57	118.32	110.14
1	A	138	HIS	N-CA-C	5.49	118.31	110.24
1	A	42	ILE	CA-C-O	5.49	122.76	119.19
1	B	168	HIS	CA-CB-CG	-5.43	108.36	113.80
1	A	70	HIS	CA-CB-CG	-5.40	108.40	113.80
1	B	230	HIS	CB-CA-C	-5.40	103.02	111.39
1	B	382	CYS	N-CA-C	-5.38	106.10	113.30
1	A	241	ALA	N-CA-C	-5.36	105.34	111.07
1	B	71	LEU	N-CA-C	5.31	117.48	111.11
1	A	88	ALA	N-CA-CB	5.27	119.21	110.52
1	A	154	ILE	N-CA-C	5.19	119.09	113.43
1	B	362	GLU	CB-CA-C	5.18	119.60	110.37
1	B	26	CYS	N-CA-CB	-5.17	102.69	111.69
1	B	69	VAL	N-CA-C	5.15	115.54	108.12
1	B	235	VAL	N-CA-C	5.15	120.01	108.88
1	B	125	GLU	CA-C-O	5.13	125.86	120.42
1	B	284	SER	N-CA-C	5.12	117.65	111.40
1	A	73	GLY	N-CA-C	-5.07	106.87	112.04
1	B	356	LEU	N-CA-C	5.05	117.48	109.50

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	2887	0	2906	111	0
1	B	2887	0	2906	76	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	9	0	3	1	0
3	B	9	0	3	0	0
4	A	129	0	0	2	0
4	B	128	0	0	0	1
All	All	6053	0	5818	182	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 16.

All (182) 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:78:ALA:HB3	1:B:82:THR:HG21	1.58	0.85
1:A:289:SER:C	1:A:291:PRO:HD3	2.06	0.81
1:A:43:PRO:HG2	1:A:46:ILE:HD13	1.66	0.77
1:A:235:VAL:HB	1:A:236:PRO:HD3	1.71	0.72
1:A:289:SER:O	1:A:291:PRO:HD3	1.90	0.72
1:B:289:SER:C	1:B:291:PRO:HD3	2.14	0.72
1:A:48:PRO:HG3	1:B:46:ILE:HG13	1.72	0.70
1:A:229:THR:HG23	1:A:230:HIS:CD2	2.27	0.70
1:B:299:LEU:HG	1:B:300:THR:N	2.08	0.68
1:A:84:THR:HB	1:A:85:PRO:HD2	1.77	0.66
1:B:235:VAL:HB	1:B:236:PRO:HD3	1.77	0.66
1:A:48:PRO:HG3	1:B:46:ILE:CG1	2.24	0.66
1:A:21:GLU:H	1:A:21:GLU:CD	2.04	0.66
1:B:289:SER:O	1:B:291:PRO:HD3	1.95	0.66
1:B:162:KCX:OQ2	1:B:201:HIS:HB2	1.97	0.65
1:A:257:ILE:O	1:A:263:PRO:HD3	1.99	0.63
1:A:290:GLN:O	1:A:302:ILE:HA	1.99	0.63
1:A:294:ASP:CG	1:A:295:ASP:H	2.06	0.62
1:B:195:PRO:HG3	1:B:340:LEU:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLU:O	1:A:269:ARG:HG3	2.00	0.62
1:B:275:ILE:HG23	1:B:276:PRO:HD2	1.83	0.61
1:A:282:LEU:HB3	1:A:332:LEU:HD21	1.82	0.61
1:A:273:ALA:HB3	1:A:275:ILE:HD12	1.82	0.61
1:A:319:LYS:HE2	1:A:320:ASP:OD1	2.02	0.60
1:B:168:HIS:CD2	1:B:169:ARG:HG3	2.37	0.60
1:B:205:SER:OG	1:B:207:LYS:HG2	2.01	0.60
1:B:43:PRO:O	1:B:46:ILE:HG22	2.03	0.59
1:A:162:KCX:OQ1	3:A:450:ASP:OD2	2.21	0.59
1:A:245:ALA:HA	1:A:249:GLY:O	2.03	0.59
1:A:27:ASP:HB2	1:A:39:ALA:O	2.03	0.59
1:A:61:CYS:HB2	1:A:62:PRO:CD	2.33	0.58
1:B:203:GLY:O	1:B:233:ARG:HD3	2.04	0.58
1:B:319:LYS:HE2	1:B:320:ASP:OD1	2.03	0.57
1:A:215:LEU:C	1:A:215:LEU:HD23	2.29	0.57
1:A:282:LEU:HB3	1:A:332:LEU:CD2	2.34	0.57
1:A:205:SER:OG	1:A:207:LYS:HD2	2.04	0.57
1:A:58:GLN:HG2	1:A:366:GLU:OE1	2.04	0.57
1:A:128:ILE:O	1:A:371:ARG:NH2	2.30	0.56
1:B:113:PRO:HB2	1:B:144:ILE:CG1	2.35	0.56
1:A:15:ALA:HB2	1:A:55:LEU:CB	2.36	0.56
1:A:367:GLN:HA	1:A:376:VAL:O	2.05	0.56
1:B:230:HIS:O	1:B:233:ARG:HG2	2.06	0.56
1:A:167:ASP:OD1	1:A:169:ARG:HB2	2.05	0.55
1:A:299:LEU:HG	1:A:300:THR:N	2.20	0.55
1:B:139:VAL:HA	1:B:140:PRO:C	2.31	0.55
1:A:162:KCX:HG2	1:A:163:CYS:N	2.20	0.55
1:A:233:ARG:HG2	1:A:237:LEU:HD23	1.88	0.55
1:A:48:PRO:HG3	1:B:46:ILE:CD1	2.38	0.54
1:A:151:ASP:HA	1:A:155:ILE:HD12	1.90	0.54
1:B:113:PRO:HB2	1:B:144:ILE:HG13	1.90	0.54
1:B:319:LYS:HG2	1:B:320:ASP:OD1	2.07	0.53
1:A:63:GLY:HA2	1:A:357:LEU:HG	1.91	0.53
1:A:249:GLY:O	1:A:279:ARG:HD2	2.08	0.53
1:A:78:ALA:HB2	1:A:299:LEU:HD22	1.91	0.52
1:A:150:LYS:O	1:A:154:ILE:HG12	2.09	0.52
1:B:290:GLN:O	1:B:302:ILE:HA	2.08	0.52
1:A:195:PRO:HB2	1:A:197:VAL:HG13	1.90	0.52
1:B:103:LEU:HD12	1:B:103:LEU:C	2.35	0.52
1:B:3:ASP:OD1	1:B:5:THR:HG23	2.10	0.52
1:A:376:VAL:HG13	1:A:380:LYS:C	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PRO:HG3	1:B:46:ILE:HD11	1.91	0.51
1:B:27:ASP:HB2	1:B:42:ILE:HG13	1.92	0.51
1:B:195:PRO:HB2	1:B:197:VAL:HG13	1.93	0.51
1:B:53:VAL:HG12	1:B:55:LEU:HD21	1.93	0.51
1:A:232:ASN:ND2	1:A:257:ILE:HB	2.26	0.50
1:A:255:SER:HA	1:A:263:PRO:HG3	1.93	0.50
1:A:145:THR:HG23	1:A:155:ILE:HD11	1.93	0.49
1:B:210:GLN:OE1	1:B:210:GLN:HA	2.12	0.49
1:B:215:LEU:C	1:B:215:LEU:HD23	2.37	0.49
1:A:139:VAL:HA	1:A:140:PRO:C	2.37	0.49
1:B:99:SER:HA	1:B:129:SER:O	2.13	0.49
1:A:15:ALA:HB2	1:A:55:LEU:HB2	1.93	0.49
1:B:317:LEU:O	1:B:321:TYR:HB2	2.12	0.49
1:A:30:VAL:HG12	1:A:31:ALA:N	2.28	0.48
1:A:15:ALA:HB2	1:A:55:LEU:HB3	1.95	0.48
1:B:348:ILE:HG12	1:B:356:LEU:CD2	2.43	0.48
1:A:68:HIS:HD2	1:A:285:ASP:HA	1.79	0.48
1:A:244:PHE:CE2	1:A:249:GLY:HA3	2.49	0.48
1:B:60:LEU:HD12	1:B:357:LEU:O	2.13	0.48
1:A:148:VAL:O	1:A:152:VAL:HG23	2.13	0.48
1:A:43:PRO:O	1:A:46:ILE:HG22	2.13	0.48
1:B:210:GLN:N	1:B:211:PRO:CD	2.78	0.47
1:A:58:GLN:HB3	1:A:359:MET:O	2.15	0.47
1:B:379:GLY:O	1:B:380:LYS:HG3	2.15	0.47
1:A:345:LYS:NZ	1:A:353:ASP:OD2	2.47	0.47
1:B:257:ILE:O	1:B:263:PRO:HD3	2.15	0.47
1:A:373:LYS:O	1:A:375:MET:HG2	2.14	0.47
1:B:362:GLU:H	1:B:362:GLU:CD	2.22	0.47
1:B:210:GLN:N	1:B:211:PRO:HD2	2.30	0.47
1:B:167:ASP:OD1	1:B:169:ARG:N	2.45	0.47
1:B:178:LEU:HB3	1:B:215:LEU:HD12	1.96	0.47
1:B:263:PRO:O	1:B:267:ILE:HG13	2.15	0.47
1:B:349:LEU:O	1:B:350:PRO:C	2.55	0.46
1:A:13:GLN:HA	1:A:27:ASP:OD1	2.16	0.46
1:B:61:CYS:SG	1:B:359:MET:HE2	2.56	0.46
1:A:18:TYR:C	1:A:20:PRO:HA	2.40	0.46
1:A:210:GLN:N	1:A:211:PRO:CD	2.78	0.46
1:B:209:LEU:C	1:B:211:PRO:HD2	2.41	0.46
1:A:312:GLU:O	1:A:316:VAL:HG23	2.16	0.46
1:A:67:GLN:HA	1:A:101:VAL:HB	1.98	0.45
1:A:235:VAL:CB	1:A:236:PRO:HD3	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:CYS:C	1:A:348:ILE:HD11	2.41	0.45
1:A:48:PRO:O	1:A:49:ASN:C	2.58	0.45
1:B:360:THR:OG1	1:B:362:GLU:OE1	2.33	0.45
1:A:88:ALA:O	1:A:89:LEU:C	2.59	0.45
1:A:203:GLY:O	1:A:233:ARG:HD3	2.17	0.45
1:B:29:LEU:CD2	1:B:36:ILE:HD11	2.47	0.45
1:B:235:VAL:N	1:B:236:PRO:HD2	2.32	0.45
1:A:62:PRO:N	1:A:348:ILE:HD11	2.32	0.44
1:A:83:ARG:HD3	4:A:403:HOH:O	2.18	0.44
1:A:172:ALA:N	1:A:173:PRO:CD	2.80	0.44
1:A:30:VAL:HG13	1:A:34:LYS:O	2.17	0.44
1:A:240:GLN:O	1:A:243:GLU:HG3	2.18	0.44
1:A:30:VAL:CG1	1:A:31:ALA:N	2.81	0.44
1:B:245:ALA:HA	1:B:249:GLY:O	2.17	0.44
1:A:3:ASP:OD1	1:A:5:THR:OG1	2.30	0.44
1:B:67:GLN:HA	1:B:101:VAL:HB	2.00	0.44
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.80	0.44
1:B:275:ILE:CG2	1:B:276:PRO:HD2	2.45	0.44
1:A:237:LEU:O	1:A:238:PHE:C	2.60	0.43
1:A:11:LEU:HD12	1:A:28:VAL:O	2.18	0.43
1:A:145:THR:CG2	1:A:155:ILE:HD11	2.48	0.43
1:A:178:LEU:HD23	1:A:178:LEU:HA	1.61	0.43
1:A:291:PRO:HB3	1:A:302:ILE:HD12	1.99	0.43
1:B:43:PRO:C	1:B:45:ASP:H	2.27	0.43
1:B:58:GLN:HG2	1:B:366:GLU:OE1	2.19	0.43
1:B:355:ASP:C	1:B:356:LEU:HG	2.43	0.43
1:B:332:LEU:HA	1:B:332:LEU:HD23	1.80	0.43
1:A:19:ALA:N	1:A:20:PRO:C	2.77	0.43
1:A:88:ALA:O	1:A:91:ARG:HB2	2.18	0.43
1:B:244:PHE:CE2	1:B:249:GLY:HA3	2.54	0.43
1:A:78:ALA:HB3	1:A:82:THR:HG21	1.99	0.43
1:A:275:ILE:HA	1:A:276:PRO:HD3	1.90	0.43
1:B:210:GLN:NE2	1:B:214:ASP:OD1	2.50	0.43
1:A:136:ALA:O	1:A:137:TYR:C	2.60	0.43
1:A:289:SER:HA	1:A:303:GLY:O	2.19	0.43
1:A:357:LEU:CD2	1:A:368:VAL:HG22	2.48	0.43
1:A:68:HIS:CD2	1:A:285:ASP:HA	2.54	0.42
1:A:112:HIS:CD2	1:A:112:HIS:N	2.87	0.42
1:A:84:THR:HB	1:A:85:PRO:CD	2.47	0.42
1:A:210:GLN:NE2	1:A:214:ASP:OD1	2.52	0.42
1:B:359:MET:HA	1:B:364:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:HG	1:A:300:THR:H	1.84	0.42
1:B:311:LEU:O	1:B:312:GLU:C	2.59	0.42
1:A:12:LEU:HD23	1:A:53:VAL:HB	2.01	0.42
1:B:167:ASP:OD1	1:B:169:ARG:HB2	2.19	0.42
1:A:87:VAL:HG11	1:A:92:LEU:HD11	2.01	0.42
1:A:209:LEU:C	1:A:211:PRO:HD2	2.44	0.42
1:A:360:THR:HB	1:A:361:PRO:HD2	2.00	0.42
1:A:46:ILE:HG13	1:B:48:PRO:HG3	2.01	0.42
1:A:255:SER:HB3	1:A:282:LEU:HD11	2.02	0.42
1:B:245:ALA:HB3	1:B:275:ILE:HD13	2.01	0.41
1:B:235:VAL:N	1:B:236:PRO:CD	2.82	0.41
1:A:271:VAL:CG2	1:A:277:LEU:HD21	2.51	0.41
1:B:47:VAL:HB	1:B:48:PRO:HD2	2.02	0.41
1:B:271:VAL:O	1:B:274:GLY:N	2.33	0.41
1:A:61:CYS:HB2	1:A:62:PRO:HD3	2.02	0.41
1:A:254:THR:HG22	1:A:256:SER:H	1.85	0.41
1:A:321:TYR:O	1:A:322:ASP:HB2	2.20	0.41
1:B:209:LEU:O	1:B:210:GLN:C	2.63	0.41
1:B:308:GLU:HG2	1:B:309:THR:N	2.34	0.41
1:A:68:HIS:O	1:A:285:ASP:HA	2.21	0.41
1:A:299:LEU:HD11	1:A:302:ILE:HB	2.03	0.41
1:A:210:GLN:N	1:A:211:PRO:HD2	2.36	0.41
1:A:290:GLN:N	1:A:303:GLY:O	2.50	0.41
1:A:329:LEU:HD23	1:A:329:LEU:HA	1.88	0.41
1:B:43:PRO:C	1:B:45:ASP:N	2.79	0.41
1:B:166:SER:HB3	1:B:205:SER:HB3	2.03	0.41
1:B:312:GLU:O	1:B:316:VAL:HG23	2.20	0.41
1:A:370:ALA:O	1:A:371:ARG:C	2.60	0.41
1:A:57:GLY:HA3	4:A:502:HOH:O	2.21	0.40
1:B:123:LEU:HD23	1:B:123:LEU:HA	1.82	0.40
1:B:227:LEU:HB2	1:B:339:PHE:CZ	2.56	0.40
1:A:111:ARG:C	1:A:112:HIS:CD2	2.99	0.40
1:A:377:LYS:O	1:A:378:ASP:C	2.64	0.40
1:B:271:VAL:C	1:B:273:ALA:N	2.79	0.40
1:A:103:LEU:HD12	1:A:103:LEU:C	2.47	0.40
1:B:172:ALA:N	1:B:173:PRO:CD	2.85	0.40
1:A:17:LEU:HD13	1:A:60:LEU:HD23	2.04	0.40
1:A:157:ARG:HA	1:A:157:ARG:HD2	1.84	0.40
1:B:138:HIS:ND1	1:B:140:PRO:O	2.42	0.40
1:B:299:LEU:HG	1:B:300:THR:H	1.83	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:493:HOH:O	4:B:493:HOH:O[7_556]	2.13	0.07

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	387/390 (99%)	356 (92%)	29 (8%)	2 (0%)	24	22
1	B	387/390 (99%)	363 (94%)	23 (6%)	1 (0%)	36	36
All	All	774/780 (99%)	719 (93%)	52 (7%)	3 (0%)	30	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	ASP
1	A	19	ALA
1	B	44	SER

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	313/312 (100%)	296 (95%)	17 (5%)	20	18
1	B	313/312 (100%)	302 (96%)	11 (4%)	32	35
All	All	626/624 (100%)	598 (96%)	28 (4%)	24	25

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	40	SER
1	A	44	SER
1	A	109	ILE
1	A	165	ILE
1	A	201	HIS
1	A	207	LYS
1	A	210	GLN
1	A	226	LEU
1	A	240	GLN
1	A	243	GLU
1	A	299	LEU
1	A	300	THR
1	A	302	ILE
1	A	324	SER
1	A	326	SER
1	A	362	GLU
1	B	12	LEU
1	B	13	GLN
1	B	40	SER
1	B	44	SER
1	B	58	GLN
1	B	109	ILE
1	B	201	HIS
1	B	212	ILE
1	B	299	LEU
1	B	326	SER
1	B	362	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	68	HIS
1	A	112	HIS
1	A	230	HIS
1	A	315	GLN
1	A	367	GLN
1	B	13	GLN
1	B	168	HIS
1	B	240	GLN

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Mol	Chain	Res	Type
1	B	367	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	A	162	2,1	10,11,12	2.64	2 (20%)	6,12,14	3.74	2 (33%)
1	KCX	B	162	2,1	10,11,12	2.77	2 (20%)	6,12,14	4.59	2 (33%)

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	2,1	-	3/9/10/12	-
1	KCX	B	162	2,1	-	3/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	KCX	CX-NZ	6.65	1.47	1.35
1	A	162	KCX	CX-NZ	6.56	1.46	1.35
1	B	162	KCX	OQ1-CX	5.24	1.31	1.21
1	A	162	KCX	OQ1-CX	4.72	1.30	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	KCX	OQ1-CX-NZ	-8.92	111.37	124.92
1	A	162	KCX	OQ1-CX-NZ	-7.14	114.08	124.92
1	B	162	KCX	CE-NZ-CX	-6.81	110.43	121.98
1	A	162	KCX	CE-NZ-CX	-5.70	112.31	121.98

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	ASP	B	550	2	7,8,8	1.32	1 (14%)	6,10,10	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ASP	A	450	2	7,8,8	1.57	1 (14%)	6,10,10	1.56	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
3	ASP	B	550	2	-	6/8/8/8	-
3	ASP	A	450	2	-	6/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	450	ASP	CA-N	-2.90	1.33	1.48
3	B	550	ASP	CA-N	-2.56	1.35	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	450	ASP	OD2-CG-OD1	2.85	130.66	123.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	450	ASP	O-C-CA-N
3	B	550	ASP	O-C-CA-N
3	A	450	ASP	OXT-C-CA-N
3	B	550	ASP	OXT-C-CA-N
3	A	450	ASP	N-CA-CB-CG
3	B	550	ASP	N-CA-CB-CG
3	A	450	ASP	C-CA-CB-CG
3	B	550	ASP	C-CA-CB-CG
3	B	550	ASP	OXT-C-CA-CB
3	A	450	ASP	OXT-C-CA-CB
3	A	450	ASP	O-C-CA-CB
3	B	550	ASP	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	450	ASP	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	388/390 (99%)	-0.44	7 (1%) 67 70	14, 29, 66, 97	1 (0%)
1	B	388/390 (99%)	-0.48	11 (2%) 55 57	12, 28, 64, 100	1 (0%)
All	All	776/780 (99%)	-0.46	18 (2%) 61 64	12, 28, 65, 100	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299	LEU	4.3
1	B	292	PHE	4.2
1	A	292	PHE	3.6
1	A	299	LEU	3.5
1	B	297	GLY	3.2
1	A	293	PHE	2.9
1	B	389	THR	2.8
1	A	389	THR	2.7
1	B	293	PHE	2.6
1	B	295	ASP	2.6
1	A	301	HIS	2.5
1	A	1	MET	2.5
1	A	291	PRO	2.4
1	B	1	MET	2.4
1	B	290	GLN	2.3
1	B	298	ASN	2.3
1	B	301	HIS	2.2
1	B	302	ILE	2.1

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($\text{\AA}^2$)	Q<0.9
1	KCX	B	162	12/13	0.97	0.08	8,30,45,52	0
1	KCX	A	162	12/13	0.98	0.07	17,32,53,71	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
3	ASP	A	450	9/9	0.92	0.11	27,36,70,87	0
3	ASP	B	550	9/9	0.94	0.12	30,43,54,100	0
2	ZN	A	402	1/1	0.98	0.06	52,52,52,52	0
2	ZN	B	502	1/1	0.99	0.05	45,45,45,45	0
2	ZN	A	401	1/1	0.99	0.04	51,51,51,51	0
2	ZN	B	501	1/1	0.99	0.05	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.