



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:38 AM UTC

PDB ID : 3ZUU / pdb_00003zuu
Title : The structure of OST1 (D160A, S175D) kinase in complex with gold
Authors : Yunta, C.; Martinez-Ripoll, M.; Albert, A.
Deposited on : 2011-07-20
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)	:	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

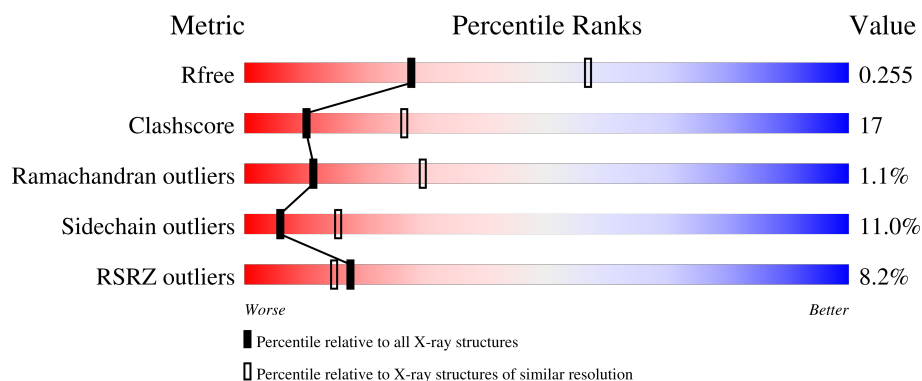
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	362	7% 51% 22% • 22%
1	B	362	6% 47% 24% 6% • 22%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4579 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 Serine/threonine-protein kinase SRK2E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2258	1444	393	409	12			
1	B	282	Total	C	N	O	S	0	0	0
			2264	1449	394	409	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	ALA	ASP	conflict	UNP Q940H6
A	175	ASP	SER	conflict	UNP Q940H6
B	160	ALA	ASP	conflict	UNP Q940H6
B	175	ASP	SER	conflict	UNP Q940H6

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is GOLD ION (CCD ID: AU) (formula: Au).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Au 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	31	Total O 31 31	0	0
4	B	17	Total O 17 17	0	0

- Molecule 1: Serine/threonine-protein kinase SRK2E



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	77.57Å 99.02Å 108.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.23 – 2.70 54.23 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (54.23-2.70) 99.9 (54.23-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.238 , 0.279 (Not available) , 0.255	Depositor DCC
R_{free} test set	1007 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.1	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	0.93	EDS
Total number of atoms	4579	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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: AU, EDO

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	0.64	0/2310	0.95	3/3125 (0.1%)
1	B	0.59	0/2316	0.94	5/3134 (0.2%)
All	All	0.62	0/4626	0.95	8/6259 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	PRO	N-CA-C	5.83	117.82	110.70
1	B	12	LEU	CA-C-N	5.73	125.64	119.85
1	B	12	LEU	C-N-CA	5.73	125.64	119.85
1	A	317	VAL	N-CA-C	5.60	114.12	107.73
1	B	52	ILE	CB-CA-C	-5.49	104.20	110.73
1	B	177	VAL	CB-CA-C	-5.34	104.29	110.91
1	B	140	ASP	N-CA-C	-5.26	106.70	113.23
1	A	79	ARG	N-CA-C	5.25	118.78	109.96

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	CYS	Peptide
1	A	318	PRO	Peptide

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	2258	0	2253	68	1
1	B	2264	0	2265	87	1
2	A	4	0	6	0	0
2	B	4	0	6	2	0
3	A	1	0	0	0	0
4	A	31	0	0	7	0
4	B	17	0	0	0	0
All	All	4579	0	4530	155	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 17.

All (155) 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:36:ARG:HG2	1:B:38:MET:HE2	1.41	0.99
1:B:20:ARG:HH11	1:B:20:ARG:HG3	1.30	0.95
1:B:222:GLU:HB3	2:B:1320:EDO:H11	1.49	0.94
1:A:28:GLY:HA2	1:A:34:VAL:HG13	1.52	0.89
1:B:49:VAL:HG22	1:B:93:VAL:HG22	1.55	0.86
1:A:55:GLY:HA2	1:A:316:THR:O	1.78	0.83
1:A:313:ALA:O	1:A:316:THR:OG1	1.97	0.82
1:A:137:CYS:SG	4:A:2014:HOH:O	2.39	0.80
1:A:39:ARG:HE	1:A:44:ASN:HA	1.48	0.78
1:B:20:ARG:HH11	1:B:20:ARG:CG	2.00	0.75
1:A:23:LEU:HD12	1:A:24:VAL:N	2.01	0.75
1:B:305:ILE:O	1:B:309:MET:HG2	1.88	0.73
1:B:222:GLU:HB3	2:B:1320:EDO:C1	2.18	0.72
1:B:43:SER:OG	1:B:45:GLU:HB2	1.91	0.71
1:A:307:GLU:O	1:A:311:ILE:HG13	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LYS:HE2	1:A:232:ARG:NH2	2.06	0.70
1:B:36:ARG:CG	1:B:38:MET:HE2	2.22	0.69
1:B:45:GLU:OE1	1:B:81:LYS:NZ	2.25	0.69
1:A:85:LEU:HD12	1:A:315:ALA:HB2	1.74	0.68
1:B:228:LYS:HE2	1:B:232:ARG:NH2	2.10	0.67
1:B:57:LYS:O	1:B:59:ASP:N	2.27	0.66
1:A:72:LEU:O	4:A:2003:HOH:O	2.13	0.66
1:B:136:VAL:HG12	1:B:140:ASP:HB2	1.77	0.66
1:A:15:MET:HA	1:A:36:ARG:HH12	1.60	0.65
1:A:24:VAL:HG21	1:A:46:LEU:HD11	1.78	0.65
1:A:262:PRO:O	4:A:2030:HOH:O	2.15	0.65
1:A:83:VAL:HG22	1:A:90:LEU:HD11	1.79	0.64
1:A:109:ALA:O	4:A:2009:HOH:O	2.15	0.64
1:B:54:ARG:HH21	1:B:319:PRO:HD3	1.62	0.64
1:B:69:HIS:CD2	1:B:80:PHE:HB2	2.33	0.63
1:B:70:ARG:NH2	1:B:303:GLN:O	2.32	0.63
1:B:92:ILE:HD13	1:B:163:TYR:CE2	2.34	0.62
1:B:28:GLY:HA2	1:B:34:VAL:HA	1.82	0.62
1:A:21:TYR:HE1	1:A:40:ASP:HB2	1.64	0.62
1:A:82:GLU:OE2	1:A:84:ILE:HD11	1.99	0.62
1:B:304:SER:HB2	1:B:306:GLU:OE1	2.00	0.61
1:A:144:GLU:H	1:A:144:GLU:CD	2.08	0.61
1:A:63:LYS:O	1:A:67:ILE:HG12	2.02	0.60
1:B:63:LYS:O	1:B:67:ILE:HG12	2.00	0.60
1:A:24:VAL:HG21	1:A:46:LEU:CD1	2.33	0.59
1:A:84:ILE:HB	1:A:91:ALA:HB3	1.85	0.58
1:A:36:ARG:HD2	1:A:38:MET:CE	2.34	0.58
1:B:151:SER:OG	1:B:153:ALA:O	2.15	0.58
1:B:188:LEU:HD13	1:B:230:ILE:HG23	1.86	0.58
1:B:92:ILE:HD13	1:B:163:TYR:CD2	2.38	0.58
1:A:23:LEU:HD12	1:A:23:LEU:C	2.28	0.57
1:B:181:ALA:HA	1:B:233:ILE:HD11	1.86	0.57
1:B:54:ARG:NH2	1:B:319:PRO:HD3	2.19	0.57
1:B:31:ASN:N	1:B:31:ASN:HD22	2.03	0.57
1:A:21:TYR:CE1	1:A:40:ASP:HB2	2.40	0.57
1:A:43:SER:O	1:A:44:ASN:CB	2.52	0.57
1:A:61:ASN:O	1:A:65:GLU:HB2	2.04	0.56
1:B:307:GLU:O	1:B:311:ILE:HG13	2.05	0.56
1:A:191:LYS:N	1:A:191:LYS:HE3	2.19	0.56
1:B:307:GLU:O	1:B:311:ILE:CG1	2.53	0.56
1:A:40:ASP:OD1	1:A:43:SER:N	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LEU:HG	1:B:13:PRO:HD2	1.89	0.55
1:B:58:ILE:HG13	1:B:316:THR:HA	1.88	0.54
1:B:74:HIS:CE1	1:B:76:ASN:HB2	2.41	0.54
1:A:42:GLN:N	1:A:42:GLN:OE1	2.39	0.54
1:A:68:ASN:O	1:A:71:SER:OG	2.23	0.54
1:B:75:PRO:HA	1:B:79:ARG:NH1	2.23	0.54
1:A:12:LEU:H	1:A:12:LEU:HD12	1.73	0.54
1:B:54:ARG:HA	1:B:58:ILE:HD11	1.89	0.54
1:B:68:ASN:O	1:B:71:SER:OG	2.22	0.53
1:B:65:GLU:OE2	1:B:163:TYR:HD1	1.91	0.53
1:A:28:GLY:O	1:A:34:VAL:HG22	2.08	0.53
1:B:31:ASN:N	1:B:31:ASN:ND2	2.56	0.53
1:B:268:ILE:HB	1:B:269:PRO:HD3	1.91	0.53
1:A:36:ARG:HD2	1:A:38:MET:HE3	1.90	0.53
1:A:268:ILE:HB	1:A:269:PRO:HD3	1.91	0.52
1:B:59:ASP:OD1	1:B:61:ASN:ND2	2.42	0.52
1:A:179:THR:N	4:A:2021:HOH:O	2.41	0.52
1:B:308:ILE:O	1:B:312:ILE:HG13	2.10	0.52
1:A:15:MET:HA	1:A:36:ARG:NH1	2.22	0.51
1:A:216:PRO:O	1:A:218:GLU:N	2.41	0.51
1:B:216:PRO:O	1:B:218:GLU:N	2.43	0.51
1:B:31:ASN:ND2	1:B:31:ASN:H	2.08	0.51
1:B:304:SER:HB2	1:B:306:GLU:CD	2.35	0.51
1:A:191:LYS:H	1:A:191:LYS:CE	2.24	0.51
1:B:92:ILE:HG21	1:B:163:TYR:HE2	1.76	0.50
1:A:236:VAL:HG12	1:A:236:VAL:O	2.11	0.50
1:B:20:ARG:HG3	1:B:20:ARG:NH1	2.10	0.50
1:B:206:THR:O	1:B:209:VAL:HG12	2.11	0.50
1:B:16:HIS:NE2	1:B:51:TYR:OH	2.30	0.49
1:B:144:GLU:H	1:B:144:GLU:CD	2.20	0.49
1:A:17:ASP:C	1:A:19:ASP:H	2.21	0.49
1:B:155:ARG:CG	1:B:155:ARG:HH11	2.26	0.48
1:B:88:THR:HB	1:B:89:HIS:ND1	2.28	0.48
1:B:88:THR:HB	1:B:89:HIS:CE1	2.47	0.48
1:A:43:SER:O	4:A:2001:HOH:O	2.20	0.48
1:B:38:MET:HE3	1:B:38:MET:HB2	1.70	0.48
1:B:236:VAL:HG12	1:B:236:VAL:O	2.14	0.48
1:B:140:ASP:HB3	1:B:161:PHE:CE1	2.48	0.48
1:A:314:GLU:O	1:A:317:VAL:HG22	2.13	0.48
1:B:58:ILE:HB	1:B:316:THR:HG23	1.95	0.48
1:B:142:LYS:HA	1:B:144:GLU:OE2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:PHE:O	1:B:50:LYS:HE3	2.14	0.47
1:B:43:SER:HG	1:B:45:GLU:HB2	1.77	0.47
1:A:74:HIS:CE1	1:A:76:ASN:HB2	2.49	0.47
1:B:280:ASN:O	1:B:282:PRO:HD3	2.15	0.47
1:A:241:PRO:HB2	1:A:244:VAL:HG23	1.96	0.47
1:B:22:GLU:OE1	1:B:39:ARG:NH2	2.44	0.47
1:A:43:SER:O	1:A:44:ASN:HB3	2.14	0.47
1:B:75:PRO:C	1:B:77:ILE:H	2.23	0.47
1:A:74:HIS:CG	1:A:75:PRO:HD2	2.50	0.46
1:B:38:MET:CE	1:B:49:VAL:HG21	2.44	0.46
1:B:85:LEU:HB2	1:B:311:ILE:HG22	1.97	0.46
1:A:136:VAL:HG12	1:A:140:ASP:HB2	1.96	0.46
1:A:54:ARG:NH2	1:A:85:LEU:HD21	2.31	0.46
1:B:52:ILE:O	1:B:53:GLU:C	2.58	0.46
1:A:280:ASN:O	1:A:282:PRO:HD3	2.16	0.46
1:B:138:HIS:HA	1:B:199:ASP:OD1	2.15	0.46
1:B:241:PRO:HB2	1:B:244:VAL:HG23	1.98	0.46
1:B:13:PRO:HB3	1:B:89:HIS:CE1	2.51	0.45
1:B:69:HIS:CD2	1:B:80:PHE:CB	2.99	0.45
1:B:14:ILE:HG13	1:B:15:MET:N	2.30	0.45
1:A:191:LYS:H	1:A:191:LYS:NZ	2.15	0.45
1:A:58:ILE:HG13	1:A:315:ALA:O	2.16	0.44
1:A:149:ASP:OD1	1:A:151:SER:HB2	2.18	0.44
1:A:182:TYR:HA	1:A:205:VAL:HG21	1.98	0.44
1:A:112:PHE:O	4:A:2011:HOH:O	2.21	0.44
1:A:54:ARG:HD3	1:A:315:ALA:HA	2.00	0.44
1:A:206:THR:O	1:A:209:VAL:HG12	2.17	0.44
1:B:51:TYR:HA	1:B:90:LEU:O	2.17	0.44
1:A:21:TYR:HA	1:A:39:ARG:O	2.18	0.44
1:B:58:ILE:H	1:B:58:ILE:HG12	1.53	0.44
1:A:25:LYS:HG3	1:A:26:ASP:N	2.33	0.43
1:B:49:VAL:HG12	1:B:51:TYR:CE1	2.53	0.43
1:A:59:ASP:OD1	1:A:59:ASP:C	2.62	0.43
1:B:62:VAL:HG12	1:B:63:LYS:N	2.33	0.43
1:B:38:MET:HE1	1:B:49:VAL:HG21	1.99	0.43
1:A:86:THR:OG1	1:A:89:HIS:N	2.45	0.43
1:B:83:VAL:HG12	1:B:311:ILE:HD12	2.00	0.43
1:B:61:ASN:O	1:B:64:ARG:HB2	2.18	0.43
1:A:14:ILE:O	1:A:15:MET:C	2.62	0.42
1:B:61:ASN:HA	1:B:64:ARG:HD3	2.00	0.42
1:B:21:TYR:HB3	1:B:38:MET:HG2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:HE	1:B:73:ARG:HB3	1.63	0.42
1:A:39:ARG:HE	1:A:44:ASN:CA	2.27	0.42
1:B:43:SER:C	1:B:45:GLU:N	2.78	0.42
1:A:267:SER:OG	1:A:269:PRO:HD2	2.20	0.42
1:A:68:ASN:HB3	1:A:161:PHE:CZ	2.55	0.41
1:B:267:SER:O	1:B:271:ILE:HG13	2.20	0.41
1:B:53:GLU:HA	1:B:89:HIS:CD2	2.55	0.41
1:A:305:ILE:O	1:A:305:ILE:HG13	2.20	0.41
1:B:72:LEU:C	1:B:73:ARG:HG2	2.46	0.41
1:B:20:ARG:CG	1:B:20:ARG:NH1	2.67	0.41
1:B:307:GLU:O	1:B:311:ILE:HG12	2.20	0.41
1:B:267:SER:OG	1:B:269:PRO:HD2	2.21	0.41
1:A:197:VAL:HG12	1:A:265:ARG:NH1	2.35	0.40
1:B:149:ASP:OD1	1:B:149:ASP:C	2.63	0.40
1:A:191:LYS:N	1:A:191:LYS:CE	2.82	0.40
1:B:118:ARG:HD3	1:B:276:TRP:O	2.22	0.40
1:A:23:LEU:HD13	1:A:36:ARG:HD3	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)
1:A:190:LYS:O	1:B:227:ARG:NH2[3_655]	2.11	0.09

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	275/362 (76%)	252 (92%)	21 (8%)	2 (1%)	18	41
1	B	276/362 (76%)	246 (89%)	26 (9%)	4 (1%)	9	23
All	All	551/724 (76%)	498 (90%)	47 (8%)	6 (1%)	11	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	58	ILE
1	B	53	GLU
1	A	161	PHE
1	B	161	PHE
1	A	58	ILE
1	B	318	PRO

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	246/321 (77%)	224 (91%)	22 (9%)	9	23
1	B	247/321 (77%)	215 (87%)	32 (13%)	4	10
All	All	493/642 (77%)	439 (89%)	54 (11%)	6	15

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	18	SER
1	A	23	LEU
1	A	27	ILE
1	A	31	ASN
1	A	36	ARG
1	A	37	LEU
1	A	39	ARG
1	A	41	LYS
1	A	52	ILE
1	A	53	GLU
1	A	65	GLU
1	A	88	THR
1	A	92	ILE
1	A	115	ASP
1	A	137	CYS
1	A	190	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	191	LYS
1	A	227	ARG
1	A	284	ASP
1	A	305	ILE
1	A	316	THR
1	B	14	ILE
1	B	19	ASP
1	B	20	ARG
1	B	29	SER
1	B	31	ASN
1	B	34	VAL
1	B	37	LEU
1	B	38	MET
1	B	42	GLN
1	B	45	GLU
1	B	52	ILE
1	B	58	ILE
1	B	68	ASN
1	B	81	LYS
1	B	82	GLU
1	B	83	VAL
1	B	92	ILE
1	B	115	ASP
1	B	136	VAL
1	B	137	CYS
1	B	139	ARG
1	B	155	ARG
1	B	191	LYS
1	B	222	GLU
1	B	227	ARG
1	B	284	ASP
1	B	306	GLU
1	B	307	GLU
1	B	311	ILE
1	B	314	GLU
1	B	316	THR
1	B	317	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	31	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	69	HIS
1	B	235	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is 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	$\# Z > 2$
2	EDO	A	1320	-	3,3,3	0.82	0	2,2,2	0.78	0
2	EDO	B	1320	-	3,3,3	0.85	0	2,2,2	1.00	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
2	EDO	A	1320	-	-	1/1/1/1	-
2	EDO	B	1320	-	-	1/1/1/1	-

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
2	B	1320	EDO	O1-C1-C2-O2
2	A	1320	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1320	EDO	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	281/362 (77%)	0.55	24 (8%) 16 14	43, 61, 97, 128	0
1	B	282/362 (77%)	0.74	22 (7%) 19 16	44, 65, 114, 133	0
All	All	563/724 (77%)	0.65	46 (8%) 17 15	43, 63, 110, 133	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	ASP	6.1
1	B	34	VAL	4.2
1	A	10	MET	4.0
1	B	319	PRO	4.0
1	B	30	GLY	3.8
1	A	32	PHE	3.8
1	A	90	LEU	3.6
1	A	31	ASN	3.5
1	B	90	LEU	3.5
1	B	163	TYR	3.4
1	B	161	PHE	3.4
1	B	285	LEU	3.4
1	A	163	TYR	3.3
1	B	176	THR	3.3
1	A	319	PRO	3.2
1	A	91	ALA	3.2
1	B	32	PHE	3.2
1	A	301	PRO	3.2
1	B	92	ILE	3.1
1	B	317	VAL	2.9
1	A	34	VAL	2.9
1	B	136	VAL	2.8
1	B	31	ASN	2.8
1	B	301	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	56	GLU	2.7
1	B	177	VAL	2.5
1	B	282	PRO	2.5
1	A	162	GLY	2.4
1	A	35	ALA	2.4
1	A	14	ILE	2.4
1	A	285	LEU	2.3
1	B	162	GLY	2.3
1	A	318	PRO	2.3
1	A	23	LEU	2.3
1	A	283	ALA	2.2
1	A	52	ILE	2.2
1	A	30	GLY	2.1
1	B	305	ILE	2.1
1	A	33	GLY	2.1
1	B	91	ALA	2.1
1	B	309	MET	2.1
1	A	92	ILE	2.1
1	A	27	ILE	2.1
1	B	281	LEU	2.0
1	A	57	LYS	2.0
1	A	313	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	B	1320	4/4	0.71	0.19	57,58,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	1320	4/4	0.86	0.15	49,49,51,60	0
3	AU	A	1321	1/1	0.98	0.12	118,118,118,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.