



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:38 AM UTC

PDB ID : 4HGX / pdb_00004hgx
Title : Crystal structure of xylose isomerase domain containing protein (stm4435) from salmonella typhimurium lt2 with unknown ligand
Authors : Boyko, K.M.; Gorbacheva, M.A.; Korzhenevskiy, D.A.; Dorovatovsky, P.V.; Rakitina, T.V.; Lipkin, A.V.; Shumilin, I.A.; Minor, W.; Popov, V.O.
Deposited on : 2012-10-09
Resolution : 2.60 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

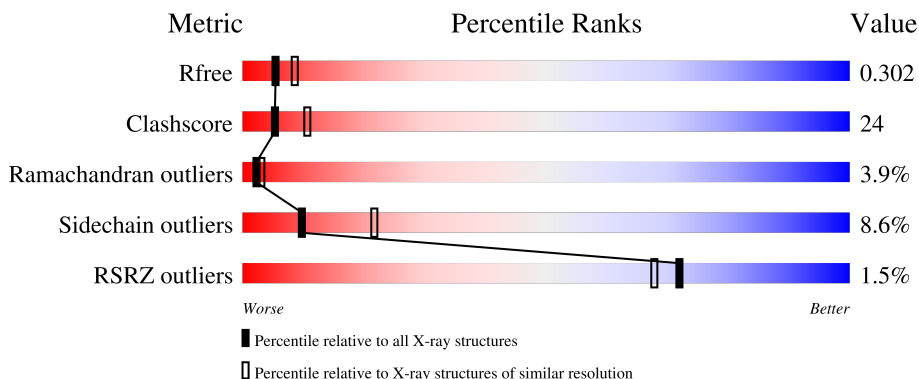
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	271	3% 51% 38% 8% ..
1	B	271	55% 37% 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4282 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 Xylose isomerase domain containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2017	1279	353	378	7			
1	B	271	Total	C	N	O	S	0	0	0
			2150	1362	372	409	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

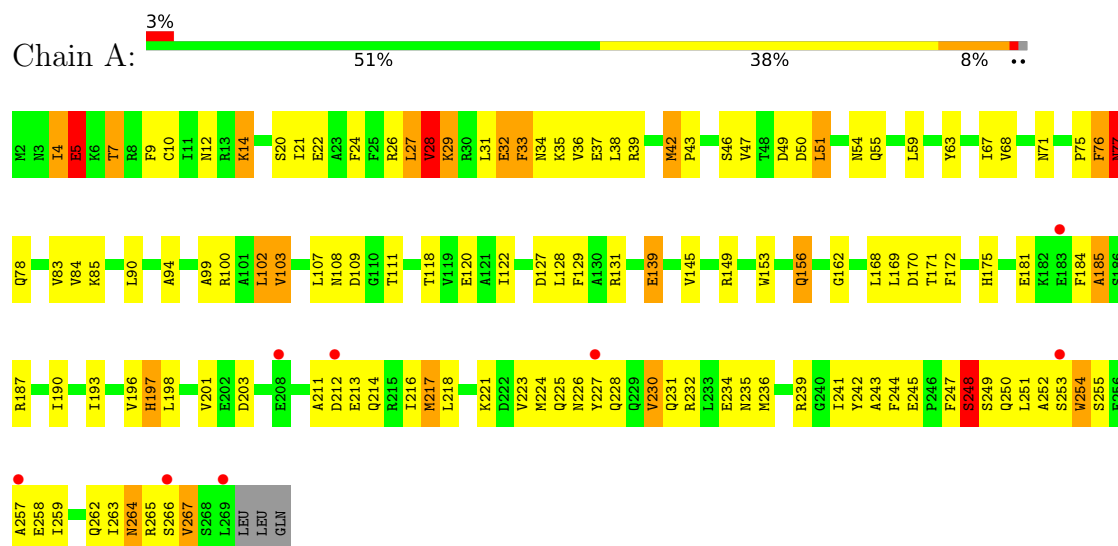
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total 37	O 37	0	0
4	B	68	Total 68	O 68	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Xylose isomerase domain containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.18Å 93.18Å 125.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.15 – 2.60 29.15 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.15-2.60) 99.4 (29.15-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.302 0.191 , 0.302	Depositor DCC
R_{free} test set	883 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.4	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	0.94	EDS
Total number of atoms	4282	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: ACT, 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	1.36	5/2053 (0.2%)	1.43	16/2794 (0.6%)
1	B	1.35	3/2187 (0.1%)	1.48	21/2960 (0.7%)
All	All	1.36	8/4240 (0.2%)	1.46	37/5754 (0.6%)

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
1	B	0	2
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	GLU	N-CA	6.03	1.53	1.46
1	B	183	GLU	N-CA	5.72	1.53	1.46
1	A	197	HIS	ND1-CE1	5.64	1.38	1.32
1	A	127	ASP	C-O	-5.58	1.17	1.24
1	B	218	LEU	CA-C	5.47	1.60	1.53
1	B	207	THR	CA-C	5.42	1.60	1.52
1	A	128	LEU	N-CA	-5.04	1.40	1.46
1	A	84	VAL	C-O	-5.02	1.18	1.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	LEU	N-CA-C	8.55	121.82	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	MET	CA-C-N	-8.12	111.27	119.56
1	B	42	MET	C-N-CA	-8.12	111.27	119.56
1	A	211	ALA	N-CA-C	7.73	119.76	108.86
1	B	105	CYS	CA-C-N	-7.59	112.86	120.98
1	B	105	CYS	C-N-CA	-7.59	112.86	120.98
1	B	155	GLN	N-CA-C	-7.56	103.02	111.71
1	A	103	VAL	N-CA-C	-7.48	97.68	108.53
1	B	114	PRO	CA-C-N	-7.23	111.08	119.47
1	B	114	PRO	C-N-CA	-7.23	111.08	119.47
1	A	77	ASN	N-CA-CB	-7.11	98.48	110.49
1	B	77	ASN	N-CA-CB	-6.90	99.62	110.46
1	A	5	GLU	N-CA-C	6.67	125.00	110.80
1	B	152	VAL	N-CA-C	-6.61	104.41	110.82
1	B	30	ARG	N-CA-C	-6.43	104.27	111.28
1	A	203	ASP	N-CA-C	6.30	119.75	110.30
1	A	36	VAL	N-CA-C	6.22	117.80	108.96
1	A	33	PHE	N-CA-C	5.98	118.60	110.35
1	A	76	PHE	CA-C-N	5.84	132.69	121.54
1	A	76	PHE	C-N-CA	5.84	132.69	121.54
1	B	192	ALA	N-CA-C	-5.78	105.42	112.88
1	B	76	PHE	CA-C-N	5.71	132.67	122.06
1	B	76	PHE	C-N-CA	5.71	132.67	122.06
1	A	139	GLU	CA-C-N	-5.70	113.89	119.76
1	A	139	GLU	C-N-CA	-5.70	113.89	119.76
1	A	77	ASN	N-CA-C	5.61	122.74	110.80
1	B	133	ASP	CB-CA-C	-5.57	103.67	111.80
1	A	102	LEU	N-CA-C	-5.53	100.88	109.72
1	B	20	SER	N-CA-C	-5.51	103.20	110.43
1	B	103	VAL	N-CA-C	-5.44	100.60	108.87
1	A	34	ASN	N-CA-C	5.38	121.67	113.61
1	A	83	VAL	N-CA-C	5.31	115.93	110.36
1	B	73	VAL	CB-CA-C	-5.23	104.36	111.15
1	A	51	LEU	N-CA-C	5.21	116.66	110.19
1	B	21	ILE	N-CA-C	5.16	116.50	110.62
1	B	4	ILE	CB-CA-C	-5.09	104.61	110.41
1	B	232	ARG	N-CA-C	-5.04	105.68	111.07

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	A	264	ASN	Peptide
1	B	2	MET	Peptide
1	B	78	GLN	Peptide

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	2017	0	1908	103	0
1	B	2150	0	2140	96	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	3	1	0
3	B	4	0	3	0	0
4	A	37	0	0	4	0
4	B	68	0	0	2	0
All	All	4282	0	4054	199	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 24.

All (199) 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:203:ASP:OD1	1:B:205:ARG:HG3	1.57	1.04
1:A:172:PHE:HA	1:A:224:MET:HE1	1.40	1.03
1:B:239:ARG:HG2	1:B:239:ARG:HH11	1.27	0.99
1:A:254:TRP:HA	1:A:258:GLU:CB	1.96	0.95
1:B:263:ILE:O	1:B:267:VAL:HG23	1.71	0.89
1:A:190:ILE:HG13	1:A:236:MET:HE2	1.53	0.88
1:A:213:GLU:O	1:A:248:SER:HB2	1.75	0.86
1:B:77:ASN:HD22	1:B:106:PRO:HB2	1.42	0.83
1:A:218:LEU:HB2	1:A:266:SER:CB	2.08	0.82
1:A:118:THR:O	1:A:122:ILE:HG13	1.79	0.81
1:B:203:ASP:OD1	1:B:205:ARG:CG	2.30	0.80
1:B:27:LEU:C	1:B:27:LEU:HD23	2.06	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HD23	1:A:28:VAL:N	1.98	0.78
1:A:55:GLN:O	1:A:59:LEU:HG	1.83	0.78
1:B:27:LEU:HD23	1:B:27:LEU:O	1.83	0.77
1:A:10:CYS:O	1:A:243:ALA:HA	1.85	0.77
1:B:175:HIS:ND1	1:B:224:MET:HE2	2.00	0.76
1:A:230:VAL:HG22	1:A:242:TYR:CE1	2.21	0.76
1:B:34:ASN:HA	1:B:65:LEU:CD2	2.16	0.76
1:A:4:ILE:HD11	1:A:9:PHE:CZ	2.21	0.76
1:B:30:ARG:NH2	1:B:256:GLU:OE1	2.22	0.73
1:B:239:ARG:HG2	1:B:239:ARG:NH1	1.96	0.73
1:B:239:ARG:HH11	1:B:239:ARG:CG	2.01	0.72
1:A:172:PHE:HA	1:A:224:MET:CE	2.19	0.71
1:B:255:SER:C	1:B:257:ALA:H	1.99	0.71
1:B:34:ASN:HA	1:B:65:LEU:HD22	1.72	0.71
1:B:77:ASN:ND2	1:B:106:PRO:HB2	2.04	0.71
1:A:175:HIS:CB	1:A:224:MET:HE2	2.21	0.70
1:B:151:ALA:O	1:B:155:GLN:HG3	1.91	0.70
1:A:225:GLN:HB3	1:A:228:GLN:HB2	1.73	0.70
1:B:31:LEU:HD22	1:B:264:ASN:HD21	1.57	0.70
1:B:31:LEU:HD21	1:B:260:GLU:HG2	1.72	0.69
1:A:263:ILE:O	1:A:263:ILE:HG22	1.92	0.68
1:A:190:ILE:CG1	1:A:236:MET:HE2	2.23	0.68
1:A:26:ARG:HA	1:A:63:TYR:CE1	2.28	0.67
1:B:169:LEU:HD12	1:B:193:ILE:HD13	1.75	0.67
1:A:14:LYS:HE3	1:A:42:MET:HE1	1.76	0.67
1:B:16:ALA:HB1	1:B:19:LEU:HG	1.77	0.67
1:B:254:TRP:CZ3	1:B:262:GLN:HG3	2.31	0.66
1:B:77:ASN:HD22	1:B:106:PRO:CB	2.09	0.66
1:A:230:VAL:HG22	1:A:242:TYR:CZ	2.31	0.66
1:A:247:PHE:O	1:A:248:SER:O	2.14	0.64
1:A:181:GLU:H	1:A:184:PHE:HB3	1.63	0.64
1:B:158:ILE:HG23	1:B:163:SER:HB3	1.79	0.64
1:B:255:SER:C	1:B:257:ALA:N	2.53	0.63
1:A:250:GLN:C	1:A:252:ALA:H	2.06	0.63
1:A:94:ALA:HB1	1:A:99:ALA:HB3	1.80	0.63
1:A:181:GLU:H	1:A:184:PHE:CB	2.12	0.62
1:B:258:GLU:O	1:B:262:GLN:HG2	2.01	0.61
1:A:175:HIS:CG	1:A:224:MET:HE2	2.36	0.61
1:B:27:LEU:C	1:B:27:LEU:CD2	2.74	0.60
1:B:181:GLU:HA	1:B:181:GLU:OE1	2.00	0.60
1:A:90:LEU:HB3	1:A:102:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:TRP:HB3	1:A:259:ILE:HG13	1.83	0.60
1:B:31:LEU:CD2	1:B:264:ASN:HD21	2.14	0.59
1:A:263:ILE:O	1:A:266:SER:O	2.21	0.59
1:B:64:GLY:O	1:B:65:LEU:HD23	2.03	0.59
1:A:217:MET:HE1	1:A:244:PHE:HB3	1.84	0.59
1:A:10:CYS:N	1:A:242:TYR:O	2.34	0.58
1:A:201:VAL:HG22	1:A:214:GLN:O	2.03	0.58
1:A:28:VAL:O	1:A:29:LYS:CB	2.51	0.58
1:A:230:VAL:O	1:A:234:GLU:HG2	2.05	0.57
1:A:217:MET:HB2	1:A:262:GLN:HG2	1.86	0.56
1:A:42:MET:CB	1:A:43:PRO:CD	2.83	0.56
1:A:230:VAL:CG2	1:A:242:TYR:CE1	2.88	0.56
1:A:226:ASN:O	1:A:230:VAL:HB	2.05	0.56
1:B:108:ASN:OD1	1:B:145:VAL:HG23	2.06	0.56
1:B:189:ASP:OD1	1:B:189:ASP:C	2.48	0.56
1:A:67:ILE:O	1:A:99:ALA:HA	2.06	0.56
1:A:31:LEU:O	1:A:32:GLU:CB	2.55	0.55
1:B:22:GLU:O	1:B:26:ARG:HB2	2.06	0.55
1:B:39:ARG:HA	1:B:71:ASN:O	2.06	0.55
1:A:12:ASN:HB3	1:A:244:PHE:O	2.06	0.55
1:A:181:GLU:CD	1:A:232:ARG:HH12	2.14	0.55
1:A:263:ILE:O	1:A:263:ILE:CG2	2.55	0.55
1:A:21:ILE:HD12	1:A:51:LEU:HD12	1.90	0.54
1:B:13:ARG:HG3	1:B:24:PHE:CD2	2.43	0.54
1:B:19:LEU:HB3	1:B:23:ALA:HB3	1.88	0.54
1:A:27:LEU:HD23	1:A:27:LEU:C	2.33	0.53
1:B:19:LEU:N	1:B:19:LEU:HD23	2.23	0.53
1:B:223:VAL:O	1:B:223:VAL:CG1	2.56	0.53
1:B:77:ASN:ND2	1:B:106:PRO:CB	2.68	0.53
1:B:18:GLY:C	1:B:19:LEU:HD23	2.34	0.52
1:B:59:LEU:HG	4:B:414:HOH:O	2.08	0.52
1:B:263:ILE:O	1:B:267:VAL:CG2	2.53	0.51
1:A:12:ASN:OD1	1:A:39:ARG:HD2	2.10	0.51
1:A:249:SER:O	1:A:252:ALA:CB	2.59	0.51
1:B:22:GLU:HG3	1:B:59:LEU:HD22	1.93	0.51
1:B:29:LYS:O	1:B:30:ARG:C	2.52	0.51
1:A:27:LEU:CD2	1:A:28:VAL:N	2.74	0.50
1:A:227:TYR:O	1:A:231:GLN:N	2.38	0.50
1:B:48:THR:HG22	1:B:56:VAL:HG21	1.94	0.50
1:A:35:LYS:HE3	1:A:241:ILE:HD11	1.93	0.50
1:B:213:GLU:HB3	1:B:214:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:HA	1:A:63:TYR:CD1	2.47	0.49
1:B:31:LEU:HD22	1:B:264:ASN:ND2	2.25	0.49
1:B:77:ASN:OD1	1:B:113:VAL:HG11	2.13	0.49
1:A:42:MET:HB2	1:A:43:PRO:HD2	1.95	0.49
1:A:254:TRP:CD1	1:A:254:TRP:N	2.79	0.49
1:A:190:ILE:HD13	1:A:193:ILE:HD12	1.92	0.49
1:B:255:SER:O	1:B:257:ALA:N	2.45	0.49
1:A:35:LYS:HB3	1:A:68:VAL:CG2	2.42	0.49
1:A:184:PHE:O	1:A:185:ALA:HB3	2.12	0.49
1:B:13:ARG:NH1	1:B:42:MET:HG3	2.27	0.49
1:B:269:LEU:O	1:B:272:GLN:HB2	2.12	0.49
1:A:102:LEU:HD23	1:A:129:PHE:CZ	2.48	0.48
1:A:12:ASN:ND2	1:A:245:GLU:HG3	2.27	0.48
1:B:218:LEU:HB2	1:B:266:SER:HA	1.96	0.48
1:A:139:GLU:OE2	1:A:170:ASP:HB2	2.14	0.48
1:A:266:SER:O	1:A:267:VAL:HB	2.13	0.48
1:A:169:LEU:HB3	1:A:196:VAL:HG22	1.95	0.48
1:A:172:PHE:HD2	1:A:224:MET:HE1	1.77	0.48
1:B:114:PRO:O	1:B:115:PRO:C	2.51	0.48
1:B:172:PHE:CE1	1:B:176:LEU:HD22	2.49	0.48
1:A:108:ASN:OD1	1:A:145:VAL:HG23	2.14	0.48
1:B:109:ASP:OD1	1:B:109:ASP:C	2.57	0.48
1:B:203:ASP:OD1	1:B:204:THR:N	2.47	0.47
1:A:20:SER:O	1:A:24:PHE:N	2.35	0.47
1:B:205:ARG:O	1:B:206:PRO:C	2.57	0.47
1:B:254:TRP:CH2	1:B:262:GLN:HG3	2.48	0.47
1:A:37:GLU:CD	1:A:197:HIS:HE2	2.21	0.47
1:B:12:ASN:O	1:B:15:ILE:HG22	2.13	0.47
1:A:212:ASP:O	1:A:247:PHE:HB2	2.15	0.47
1:B:168:LEU:HD21	1:B:197:HIS:CG	2.50	0.46
1:A:35:LYS:HB3	1:A:68:VAL:HG21	1.96	0.46
1:A:109:ASP:OD1	1:A:111:THR:OG1	2.27	0.46
1:A:184:PHE:CD1	1:A:185:ALA:N	2.83	0.46
1:A:250:GLN:C	1:A:252:ALA:N	2.72	0.46
1:B:175:HIS:HD1	1:B:224:MET:HE2	1.75	0.46
1:B:77:ASN:ND2	1:B:147:SER:OG	2.49	0.46
1:B:234:GLU:O	1:B:235:ASN:C	2.58	0.46
1:A:75:PRO:HG2	1:A:78:GLN:HB3	1.98	0.46
1:A:267:VAL:HG12	1:A:267:VAL:O	2.16	0.46
1:B:38:LEU:HB3	1:B:47:VAL:HG13	1.96	0.46
1:A:175:HIS:HB3	1:A:224:MET:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:TYR:HE1	1:B:106:PRO:O	1.99	0.46
1:A:39:ARG:HA	1:A:71:ASN:O	2.15	0.45
1:B:172:PHE:CG	1:B:215:ARG:HD2	2.51	0.45
1:B:218:LEU:O	1:B:219:SER:HB3	2.15	0.45
1:A:38:LEU:HD13	1:A:47:VAL:O	2.17	0.45
1:A:172:PHE:HD2	1:A:224:MET:CE	2.30	0.45
1:A:76:PHE:CG	1:A:77:ASN:N	2.85	0.45
1:A:249:SER:O	1:A:252:ALA:HB3	2.18	0.44
1:A:255:SER:C	1:A:257:ALA:N	2.75	0.44
1:A:168:LEU:HD11	1:A:197:HIS:CE1	2.52	0.44
1:B:205:ARG:HG3	1:B:205:ARG:H	1.25	0.44
1:B:214:GLN:CD	1:B:214:GLN:N	2.75	0.44
1:A:162:GLY:HA2	4:A:402:HOH:O	2.17	0.44
1:B:190:ILE:C	1:B:192:ALA:H	2.25	0.44
1:B:153:TRP:CZ3	1:B:156:GLN:OE1	2.71	0.44
1:A:42:MET:HB2	1:A:43:PRO:CD	2.48	0.44
1:A:5:GLU:O	1:A:7:THR:N	2.46	0.43
1:A:14:LYS:HD3	1:A:247:PHE:CD1	2.53	0.43
1:A:258:GLU:O	1:A:259:ILE:C	2.61	0.43
1:A:149:ARG:H	3:A:302:ACT:C	2.30	0.43
1:B:153:TRP:HZ3	1:B:156:GLN:OE1	2.00	0.43
1:A:21:ILE:HG13	4:A:417:HOH:O	2.18	0.43
1:A:175:HIS:CB	1:A:224:MET:CE	2.93	0.43
1:B:15:ILE:HG13	1:B:246:PRO:HG3	2.00	0.43
1:A:12:ASN:HA	1:A:37:GLU:HB2	2.01	0.43
1:B:175:HIS:CD2	1:B:224:MET:HA	2.53	0.43
1:A:217:MET:HA	1:A:217:MET:HE2	2.00	0.43
1:A:264:ASN:O	1:A:265:ARG:C	2.61	0.43
1:B:213:GLU:HB3	1:B:214:GLN:NE2	2.34	0.43
1:A:77:ASN:HD22	1:A:107:LEU:H	1.66	0.43
1:B:35:LYS:HD3	1:B:241:ILE:HD13	2.00	0.43
1:B:214:GLN:N	1:B:214:GLN:NE2	2.67	0.43
1:B:12:ASN:OD1	1:B:39:ARG:HD2	2.18	0.43
1:A:181:GLU:H	1:A:184:PHE:HB2	1.84	0.43
1:B:129:PHE:CE2	1:B:136:GLY:HA2	2.53	0.42
1:B:2:MET:HB2	1:B:3:ASN:H	1.67	0.42
1:A:100:ARG:NH2	4:A:405:HOH:O	2.52	0.42
1:A:153:TRP:O	1:A:156:GLN:HB2	2.19	0.42
1:B:236:MET:HB3	1:B:236:MET:HE2	1.70	0.42
1:B:265:ARG:O	1:B:268:SER:N	2.47	0.42
1:A:42:MET:O	1:A:43:PRO:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:GLY:C	1:B:65:LEU:HD23	2.45	0.42
1:B:175:HIS:CG	1:B:224:MET:HE2	2.54	0.42
1:A:187:ARG:NE	4:A:425:HOH:O	2.52	0.41
1:A:217:MET:CE	1:A:244:PHE:HB3	2.50	0.41
1:A:254:TRP:CB	1:A:259:ILE:HG13	2.48	0.41
1:B:107:LEU:HD21	1:B:111:THR:HB	2.02	0.41
1:B:182:LYS:NZ	1:B:182:LYS:HB2	2.35	0.41
1:A:71:ASN:OD1	1:A:103:VAL:HG21	2.20	0.41
1:B:27:LEU:HD21	1:B:31:LEU:HD11	2.01	0.41
1:B:126:SER:O	1:B:127:ASP:C	2.60	0.41
1:A:42:MET:HA	1:A:42:MET:HE2	2.03	0.41
1:B:262:GLN:O	1:B:263:ILE:C	2.62	0.41
1:B:182:LYS:NZ	4:B:460:HOH:O	2.49	0.41
1:A:201:VAL:H	1:A:224:MET:HG3	1.85	0.41
1:B:225:GLN:O	1:B:229:GLN:HG3	2.21	0.41
1:A:42:MET:CB	1:A:43:PRO:HD2	2.50	0.41
1:B:219:SER:C	1:B:221:LYS:H	2.29	0.41
1:B:101:ALA:HA	1:B:135:GLN:O	2.21	0.41
1:B:170:ASP:O	1:B:171:THR:C	2.64	0.41
1:B:219:SER:O	1:B:221:LYS:N	2.54	0.40
1:A:198:LEU:HD11	1:A:242:TYR:CD1	2.56	0.40
1:B:215:ARG:NH2	1:B:245:GLU:O	2.54	0.40
1:B:176:LEU:N	1:B:176:LEU:CD1	2.84	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	266/271 (98%)	223 (84%)	28 (10%)	15 (6%)	1	1
1	B	269/271 (99%)	245 (91%)	18 (7%)	6 (2%)	5	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	535/542 (99%)	468 (88%)	46 (9%)	21 (4%)	2 3

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	28	VAL
1	A	32	GLU
1	A	248	SER
1	A	267	VAL
1	B	207	THR
1	A	49	ASP
1	A	77	ASN
1	A	185	ALA
1	A	251	LEU
1	A	253	SER
1	B	250	GLN
1	A	50	ASP
1	A	5	GLU
1	A	29	LYS
1	B	219	SER
1	B	220	GLU
1	B	256	GLU
1	A	235	ASN
1	A	216	ILE
1	B	216	ILE

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	199/237 (84%)	179 (90%)	20 (10%)	7 15
1	B	233/237 (98%)	216 (93%)	17 (7%)	13 29
All	All	432/474 (91%)	395 (91%)	37 (9%)	10 22

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	5	GLU
1	A	7	THR
1	A	14	LYS
1	A	22	GLU
1	A	28	VAL
1	A	33	PHE
1	A	42	MET
1	A	46	SER
1	A	54	ASN
1	A	85	LYS
1	A	131	ARG
1	A	156	GLN
1	A	171	THR
1	A	217	MET
1	A	223	VAL
1	A	230	VAL
1	A	239	ARG
1	A	248	SER
1	A	254	TRP
1	B	2	MET
1	B	19	LEU
1	B	26	ARG
1	B	32	GLU
1	B	156	GLN
1	B	166	LYS
1	B	178	GLU
1	B	179	GLU
1	B	182	LYS
1	B	187	ARG
1	B	205	ARG
1	B	213	GLU
1	B	221	LYS
1	B	239	ARG
1	B	268	SER
1	B	269	LEU
1	B	272	GLN

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

Mol	Chain	Res	Type
1	A	54	ASN
1	A	77	ASN
1	A	135	GLN
1	A	156	GLN
1	A	175	HIS
1	A	262	GLN
1	B	77	ASN
1	B	95	GLN
1	B	175	HIS
1	B	214	GLN
1	B	226	ASN
1	B	264	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 4 ligands modelled in this entry, 2 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	ACT	A	302	-	3,3,3	0.82	0	3,3,3	2.02	1 (33%)
3	ACT	B	302	-	3,3,3	0.60	0	3,3,3	1.88	1 (33%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	302	ACT	OXT-C-CH3	2.76	126.62	115.05
3	B	302	ACT	OXT-C-CH3	2.59	125.90	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	ACT	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	268/271 (98%)	-0.12	8 (2%) 52 47	18, 41, 81, 101	0
1	B	271/271 (100%)	-0.72	0 100 100	15, 29, 51, 69	0
All	All	539/542 (99%)	-0.42	8 (1%) 72 68	15, 32, 74, 101	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	ASP	3.7
1	A	227	TYR	3.0
1	A	269	LEU	2.9
1	A	266	SER	2.4
1	A	257	ALA	2.3
1	A	208	GLU	2.2
1	A	183	GLU	2.1
1	A	253	SER	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
3	ACT	B	302	4/4	0.85	0.16	38,39,42,45	0
3	ACT	A	302	4/4	0.93	0.15	23,27,30,30	0
2	ZN	A	301	1/1	0.99	0.02	40,40,40,40	0
2	ZN	B	301	1/1	1.00	0.03	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.