



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 11:55 AM UTC

PDB ID : 2RJR / pdb_00002rjr
Title : Substrate mimic bound to SgTAM
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Deposited on : 2007-10-15
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

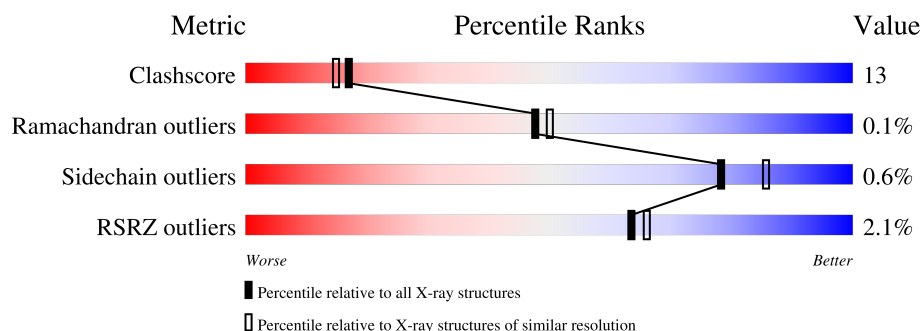
1 Overall quality at a glance

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))
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	537	2% 71% 25% ..
1	B	537	2% 79% 17% ..

2 Entry composition [i](#)

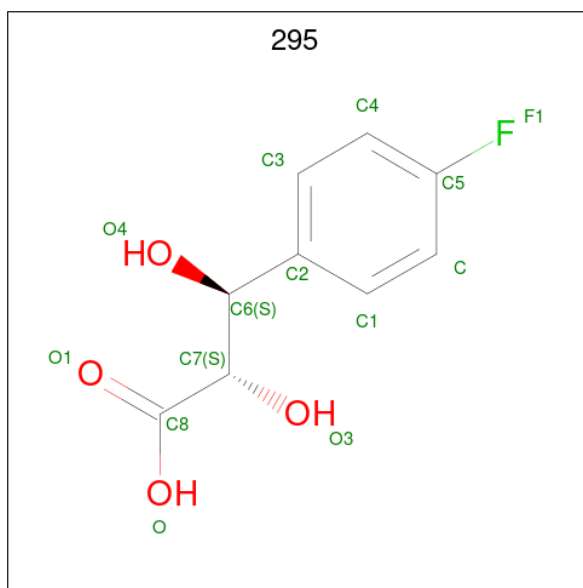
There are 3 unique types of molecules in this entry. The entry contains 8501 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tyrosine aminomutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	526	Total	C	N	O	S	0	0	0
			4007	2503	727	769	8			
1	B	526	Total	C	N	O	S	0	0	0
			4007	2503	727	769	8			

- Molecule 2 is (2S,3S)-3-(4-fluorophenyl)-2,3-dihydroxypropanoic acid (CCD ID: 295) (formula: C₉H₉FO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	O	0	0
			14	9	1	4		

- Molecule 3 is water.

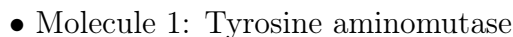
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	236	Total	O	0	0
			236	236		

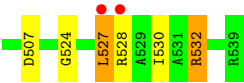
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	237	Total	O	0	0
			237	237		

- Molecule 1: Tyrosine aminomutase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.25Å 145.65Å 75.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 25.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (25.00-2.10) 95.4 (25.00-2.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.33 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.173 , 0.212 0.176 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8501	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.3260e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 295, MDO

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	0.57	8/4053 (0.2%)	0.91	11/5490 (0.2%)
1	B	0.55	8/4053 (0.2%)	0.91	10/5490 (0.2%)
All	All	0.56	16/8106 (0.2%)	0.91	21/10980 (0.2%)

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	1	0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	ASN	C-O	-10.07	1.12	1.24
1	A	47	LYS	C-O	-9.30	1.13	1.24
1	A	272	ARG	C-O	-9.15	1.12	1.23
1	B	532	ARG	C-O	-8.36	1.13	1.24
1	B	180	GLU	C-O	-7.79	1.14	1.23
1	B	532	ARG	N-CA	-7.19	1.36	1.46
1	B	292	GLU	CA-C	-7.00	1.44	1.52
1	A	46	GLN	C-O	-6.75	1.16	1.24
1	B	292	GLU	CD-OE2	-6.46	1.13	1.25
1	B	291	LYS	C-O	-6.13	1.16	1.23
1	B	292	GLU	CD-OE1	-5.67	1.14	1.25
1	A	47	LYS	N-CA	-5.64	1.39	1.46
1	A	310	LEU	CA-C	-5.52	1.45	1.52
1	A	310	LEU	C-O	-5.23	1.17	1.24
1	B	291	LYS	CE-NZ	-5.21	1.33	1.49
1	A	388	ASN	C-N	-5.18	1.27	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	ALA	N-CA-C	13.39	129.39	113.18
1	A	255	ARG	CA-C-N	7.71	129.48	119.84
1	A	255	ARG	C-N-CA	7.71	129.48	119.84
1	B	254	ALA	N-CA-C	7.53	119.57	111.36
1	A	310	LEU	N-CA-C	7.15	121.31	112.59
1	A	156	LEU	N-CA-C	6.70	119.20	111.02
1	A	47	LYS	N-CA-C	6.27	118.91	111.33
1	A	254	ALA	N-CA-C	6.19	118.11	111.36
1	B	65	VAL	N-CA-C	-6.03	106.86	111.62
1	A	511	ALA	N-CA-C	5.97	118.27	111.11
1	B	144	ILE	N-CA-C	5.72	113.72	107.60
1	B	150	LEU	N-CA-C	-5.68	105.68	113.30
1	A	144	ILE	N-CA-C	5.43	113.41	107.60
1	B	256	PRO	N-CA-C	5.38	123.56	112.47
1	B	433	GLN	N-CA-C	5.37	118.66	112.97
1	B	156	LEU	N-CA-C	5.32	117.51	111.02
1	A	146	GLU	N-CA-C	5.31	119.01	112.54
1	A	83	VAL	N-CA-C	5.29	116.06	110.72
1	A	527	LEU	N-CA-C	-5.29	105.60	111.36
1	B	406	LEU	N-CA-C	-5.13	105.69	111.28
1	B	527	LEU	N-CA-C	-5.12	105.88	111.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	537	GLN	CA

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	4007	0	4026	132	0
1	B	4007	0	4027	92	0
2	A	14	0	7	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	236	0	0	11	0
3	B	237	0	0	3	0
All	All	8501	0	8060	204	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 13.

All (204) 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:A:272:ARG:HG3	1:A:272:ARG:HH11	1.03	1.15
1:A:537:GLN:HG3	1:A:538:LEU:N	1.45	1.09
1:B:235:LEU:HD11	1:B:386:VAL:HG11	1.30	1.06
1:A:32:ARG:HH12	1:A:139:GLY:HA2	1.19	1.05
1:A:537:GLN:HG3	1:A:538:LEU:H	1.01	1.01
1:A:536:ILE:O	1:A:537:GLN:HB2	1.62	0.99
1:A:272:ARG:HG3	1:A:272:ARG:NH1	1.71	0.97
1:A:537:GLN:CG	1:A:538:LEU:H	1.77	0.96
1:A:35:VAL:H	1:A:137:ASN:HD21	1.17	0.93
1:A:272:ARG:HH11	1:A:272:ARG:CG	1.80	0.93
1:A:284:ARG:HD2	1:B:60:ILE:HD12	1.55	0.89
1:A:284:ARG:HG2	1:A:288:GLN:HE21	1.38	0.86
1:B:172:VAL:HG21	1:B:184:VAL:HG21	1.61	0.82
1:B:35:VAL:H	1:B:137:ASN:HD21	1.28	0.80
1:A:305:GLN:HE22	1:B:341:ASN:HD21	1.30	0.79
1:B:96:GLY:H	1:B:161:HIS:HE1	1.29	0.79
1:A:312:ALA:HB2	1:B:354:ALA:CB	2.14	0.77
1:A:32:ARG:NH1	1:A:139:GLY:HA2	1.97	0.76
1:B:227:GLN:CG	1:B:527:LEU:HG	2.15	0.76
1:B:172:VAL:CG2	1:B:184:VAL:HG21	2.16	0.76
1:A:125:ARG:HD3	1:A:199:GLU:OE2	1.87	0.75
1:A:536:ILE:O	1:A:537:GLN:CB	2.34	0.74
1:A:96:GLY:H	1:A:161:HIS:HE1	1.33	0.73
1:B:71:GLU:H	1:B:438:ASN:HD21	1.35	0.73
1:B:235:LEU:HD11	1:B:386:VAL:CG1	2.13	0.73
1:A:58:GLN:HB2	1:A:60:ILE:HG13	1.71	0.72
1:A:491:LYS:O	1:A:495:GLU:HG2	1.89	0.72
1:B:286:GLU:HG2	1:B:302:ILE:HD13	1.72	0.72
1:A:251:HIS:HD2	1:A:260:GLN:HE21	1.37	0.71
1:B:17:GLY:H	1:B:115:ASN:ND2	1.88	0.71
1:A:407:HIS:HD2	1:A:507:ASP:H	1.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ARG:HD2	1:B:60:ILE:CD1	2.23	0.68
1:A:537:GLN:CG	1:A:538:LEU:N	2.30	0.68
1:A:71:GLU:H	1:A:438:ASN:HD21	1.41	0.68
1:A:284:ARG:HG2	1:A:288:GLN:NE2	2.07	0.68
1:B:158:PRO:HG3	3:B:685:HOH:O	1.94	0.67
1:B:491:LYS:O	1:B:495:GLU:HG3	1.94	0.67
1:B:251:HIS:HD2	1:B:260:GLN:HE21	1.40	0.66
1:A:40:GLU:HG3	3:A:1225:HOH:O	1.95	0.66
1:A:528:ARG:HH11	1:A:528:ARG:HG3	1.61	0.66
1:B:407:HIS:HD2	1:B:507:ASP:H	1.44	0.66
1:B:49:ARG:O	1:B:53:GLU:HG3	1.96	0.66
1:B:528:ARG:NH2	3:B:626:HOH:O	2.29	0.66
1:B:227:GLN:HG2	1:B:527:LEU:HG	1.79	0.65
1:A:167:ILE:HG13	1:A:169:GLU:HG3	1.78	0.65
1:A:251:HIS:CD2	1:A:260:GLN:HE21	2.15	0.64
1:A:355:ASN:HD22	1:B:315:GLN:HE21	1.46	0.64
1:B:15:VAL:HG11	1:B:114:LEU:HG	1.80	0.64
1:A:69:TYR:CE1	1:A:85:LEU:HD11	2.33	0.64
1:B:287:LEU:HD13	1:B:302:ILE:HB	1.80	0.64
1:B:207:THR:OG1	1:B:334:GLU:OE2	2.13	0.63
1:A:305:GLN:HE21	1:B:352:HIS:HB3	1.63	0.62
1:A:60:ILE:HG23	1:A:61:PRO:HD2	1.81	0.62
1:B:286:GLU:HG2	1:B:302:ILE:CD1	2.29	0.62
1:A:355:ASN:ND2	1:B:315:GLN:HE21	1.98	0.62
1:A:281:ALA:O	1:A:285:ARG:HG3	1.99	0.61
1:A:158:PRO:HG3	3:A:1019:HOH:O	1.99	0.61
1:B:15:VAL:HG13	1:B:115:ASN:HD22	1.67	0.60
1:A:378:LEU:O	1:A:382:GLN:HG3	2.02	0.60
1:A:207:THR:H	1:A:339:ASN:HD22	1.47	0.60
1:B:124:VAL:CG2	1:B:128:ILE:HG13	2.31	0.60
1:A:475:GLN:HE21	1:A:479:ILE:HD11	1.66	0.59
1:A:93:HIS:NE2	2:A:1001:295:H4	2.17	0.59
1:B:251:HIS:CD2	1:B:260:GLN:HE21	2.20	0.59
1:A:295:LYS:HA	3:A:1121:HOH:O	2.03	0.58
1:A:296:ASP:HA	1:B:78:ASP:HB2	1.85	0.58
1:A:69:TYR:HE1	1:A:85:LEU:CD1	2.17	0.58
1:A:292:GLU:HB2	1:A:295:LYS:CE	2.34	0.58
1:A:287:LEU:HD13	1:A:302:ILE:HB	1.86	0.58
1:B:71:GLU:H	1:B:438:ASN:ND2	2.02	0.58
1:A:32:ARG:HH21	1:A:103:GLU:CD	2.11	0.57
1:A:292:GLU:HB2	1:A:295:LYS:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:PRO:HG3	1:B:479:ILE:HG21	1.86	0.57
1:A:312:ALA:HA	1:A:315:GLN:OE1	2.04	0.57
2:A:1001:295:O	2:A:1001:295:O4	2.23	0.56
3:A:1178:HOH:O	1:B:280:HIS:HE1	1.87	0.56
1:B:184:VAL:O	1:B:188:ARG:HG3	2.04	0.56
1:A:312:ALA:HB2	1:B:354:ALA:HB1	1.86	0.55
1:A:308:TYR:OH	1:B:152:MDO:HB21	2.07	0.55
1:B:330:LYS:HA	1:B:330:LYS:HE2	1.87	0.55
1:B:231:VAL:HB	1:B:470:TYR:CE1	2.42	0.55
1:B:524:GLY:O	1:B:528:ARG:HG3	2.07	0.54
1:A:74:TYR:HB2	1:B:300:SER:O	2.07	0.54
1:A:235:LEU:C	1:A:235:LEU:HD23	2.33	0.54
1:A:239:VAL:CG2	1:A:393:TYR:HB3	2.38	0.54
1:A:159:LEU:HB3	1:A:204:ILE:HA	1.90	0.53
1:A:313:ILE:HD12	1:A:313:ILE:N	2.24	0.53
1:A:96:GLY:H	1:A:161:HIS:CE1	2.21	0.52
1:A:121:HIS:HE1	3:A:1118:HOH:O	1.92	0.52
1:A:205:ASN:O	1:A:340:ASP:HA	2.09	0.52
1:A:287:LEU:HD23	1:B:61:PRO:HB3	1.91	0.52
1:B:230:ILE:CD1	1:B:527:LEU:HD23	2.40	0.52
1:B:17:GLY:H	1:B:115:ASN:HD21	1.54	0.51
1:A:232:THR:HG21	1:A:313:ILE:HG12	1.92	0.51
1:B:96:GLY:H	1:B:161:HIS:CE1	2.17	0.51
1:B:155:ASP:O	1:B:158:PRO:HD2	2.09	0.51
1:A:157:ALA:HB3	1:A:158:PRO:HD3	1.92	0.51
1:A:235:LEU:HD23	1:A:235:LEU:O	2.11	0.51
1:A:71:GLU:H	1:A:438:ASN:ND2	2.07	0.50
1:A:334:GLU:OE1	1:B:257:HIS:HE1	1.94	0.50
1:B:230:ILE:HG12	1:B:530:ILE:HD12	1.94	0.50
1:B:230:ILE:HD12	1:B:527:LEU:HD23	1.93	0.50
1:A:528:ARG:HG3	1:A:528:ARG:NH1	2.26	0.50
1:A:86:GLN:HE21	1:A:200:GLY:H	1.60	0.50
1:B:439:GLY:O	1:B:440:ASP:HB2	2.11	0.50
1:A:291:LYS:NZ	3:A:1217:HOH:O	2.43	0.50
1:A:60:ILE:CG2	1:A:61:PRO:HD2	2.41	0.50
1:A:96:GLY:HA3	1:A:145:PRO:HG2	1.93	0.49
1:B:124:VAL:HG23	1:B:199:GLU:HG2	1.94	0.49
1:A:53:GLU:O	1:A:57:GLU:HG2	2.13	0.49
1:A:183:GLN:O	1:A:187:GLU:HB2	2.12	0.49
1:A:407:HIS:CD2	1:A:507:ASP:H	2.27	0.49
1:B:152:MDO:O3	1:B:156:LEU:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:PHE:CE2	1:A:146:GLU:HG2	2.48	0.49
1:B:475:GLN:HE21	1:B:479:ILE:HD11	1.78	0.49
1:A:239:VAL:HG22	1:A:239:VAL:O	2.12	0.49
1:B:230:ILE:HG12	1:B:530:ILE:CD1	2.43	0.49
1:B:113:ARG:HD2	1:B:208:SER:OG	2.13	0.48
1:A:300:SER:O	1:B:74:TYR:HB2	2.13	0.48
1:A:286:GLU:HG2	1:A:302:ILE:HD13	1.95	0.48
1:B:101:PHE:CE2	1:B:146:GLU:HG2	2.49	0.48
1:A:93:HIS:HE2	2:A:1001:295:C5	2.28	0.47
1:A:15:VAL:HG11	1:A:114:LEU:HG	1.97	0.47
1:A:81:LYS:HZ2	1:B:296:ASP:HB3	1.79	0.47
1:A:124:VAL:CG1	1:A:128:ILE:HG13	2.45	0.47
1:A:330:LYS:HE2	1:A:330:LYS:HA	1.96	0.47
1:B:124:VAL:HG22	1:B:128:ILE:HG13	1.96	0.47
1:B:359:GLN:N	1:B:360:PRO:HD2	2.29	0.47
1:B:292:GLU:N	1:B:292:GLU:OE1	2.48	0.46
1:A:85:LEU:O	1:A:85:LEU:HD12	2.15	0.46
1:A:246:PHE:CE2	1:A:271:MET:HE1	2.50	0.46
1:A:125:ARG:HD3	1:A:199:GLU:CD	2.41	0.46
1:B:392:SER:HB2	1:B:395:LEU:HB2	1.97	0.46
1:A:225:ALA:O	1:A:229:GLU:HG3	2.15	0.46
1:B:396:PRO:CG	1:B:479:ILE:HG21	2.45	0.46
1:B:157:ALA:HB3	1:B:158:PRO:HD3	1.98	0.46
1:B:263:THR:O	1:B:267:MET:HG2	2.16	0.45
1:A:76:GLN:HB3	1:B:291:LYS:HE3	1.99	0.45
1:A:81:LYS:NZ	1:B:296:ASP:HB3	2.31	0.45
1:A:239:VAL:HG23	1:A:393:TYR:HB3	1.97	0.45
1:A:59:ASN:ND2	1:A:79:LYS:HG2	2.31	0.45
1:A:310:LEU:HA	1:A:313:ILE:HD11	1.99	0.45
3:A:1136:HOH:O	1:B:348:LYS:HE3	2.16	0.45
1:B:205:ASN:HD21	1:B:341:ASN:HB3	1.80	0.45
1:A:231:VAL:HB	1:A:470:TYR:CE1	2.52	0.45
1:A:257:HIS:HD2	1:B:330:LYS:NZ	2.14	0.45
1:A:239:VAL:HG22	1:A:393:TYR:HB3	1.99	0.45
1:A:288:GLN:HG3	1:B:61:PRO:CD	2.46	0.45
1:B:249:GLU:HG2	1:B:250:GLY:N	2.32	0.45
1:B:247:LEU:HD23	3:B:584:HOH:O	2.16	0.44
1:B:227:GLN:CG	1:B:527:LEU:CG	2.92	0.44
1:B:407:HIS:CD2	1:B:507:ASP:H	2.30	0.44
1:B:32:ARG:HD2	1:B:107:ARG:NE	2.33	0.44
1:B:205:ASN:O	1:B:340:ASP:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:NE2	2:A:1001:295:C4	2.80	0.44
1:A:244:SER:HB3	1:A:245:PRO:HD3	1.99	0.44
1:A:313:ILE:HD12	1:A:313:ILE:H	1.81	0.44
1:B:230:ILE:CD1	1:B:530:ILE:HD12	2.47	0.44
1:A:46:GLN:O	1:A:50:GLU:HG3	2.17	0.44
1:A:330:LYS:NZ	1:B:257:HIS:HD2	2.15	0.44
1:A:249:GLU:HB3	3:A:1136:HOH:O	2.17	0.44
1:A:15:VAL:HG23	1:A:35:VAL:HG13	1.99	0.44
1:A:64:GLY:HA3	1:A:201:LEU:HD22	2.00	0.44
1:A:86:GLN:HE21	1:A:200:GLY:N	2.16	0.44
1:B:392:SER:O	1:B:393:TYR:HB2	2.17	0.44
1:B:438:ASN:HD22	1:B:441:ASN:HB3	1.83	0.44
1:A:152:MDO:O3	1:A:156:LEU:N	2.49	0.44
1:B:227:GLN:HG3	1:B:527:LEU:HG	1.99	0.44
1:A:32:ARG:HH12	1:A:139:GLY:CA	2.09	0.43
1:B:125:ARG:HB3	1:B:127:ILE:HG22	2.00	0.43
1:A:442:GLN:HE21	1:A:442:GLN:HB3	1.57	0.43
1:A:508:ARG:O	1:A:509:TYR:C	2.61	0.43
1:A:101:PHE:CZ	1:A:146:GLU:HG2	2.54	0.43
1:A:196:ARG:O	1:A:197:PHE:C	2.62	0.43
1:A:344:PHE:CD1	1:A:344:PHE:C	2.97	0.43
1:A:180:GLU:O	1:A:184:VAL:HG23	2.19	0.43
1:B:15:VAL:CG1	1:B:115:ASN:HD22	2.31	0.42
1:A:285:ARG:NH1	3:A:1114:HOH:O	2.52	0.42
1:B:15:VAL:CG2	1:B:35:VAL:HG13	2.50	0.42
1:A:287:LEU:O	1:A:291:LYS:HG3	2.19	0.42
1:A:249:GLU:O	1:A:253:ILE:HB	2.20	0.42
1:A:49:ARG:NE	1:A:125:ARG:HG3	2.33	0.42
1:A:249:GLU:HG2	1:A:250:GLY:N	2.34	0.42
1:B:15:VAL:HG23	1:B:35:VAL:HG13	2.01	0.42
1:A:386:VAL:HG13	1:A:387:LEU:HD23	2.00	0.42
1:A:32:ARG:HD2	3:A:1113:HOH:O	2.18	0.42
1:A:501:VAL:HA	1:A:502:PRO:HD3	1.84	0.42
1:A:16:ASP:HB3	1:A:38:PRO:HG3	2.01	0.42
1:A:438:ASN:HD22	1:A:441:ASN:HB3	1.85	0.42
1:A:392:SER:HB2	1:A:395:LEU:HD12	2.02	0.41
1:A:230:ILE:HA	1:A:270:LEU:HD13	2.02	0.41
1:A:359:GLN:N	1:A:360:PRO:HD2	2.36	0.41
3:A:1020:HOH:O	1:B:326:HIS:HE1	2.03	0.41
1:A:32:ARG:NH2	1:A:103:GLU:CD	2.77	0.41
1:A:420:LEU:HA	1:A:420:LEU:HD23	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:LEU:O	1:A:479:ILE:HD11	2.21	0.41
1:B:125:ARG:CB	1:B:127:ILE:HG22	2.50	0.41
1:A:69:TYR:CE1	1:A:85:LEU:CD1	2.95	0.41
1:A:69:TYR:HE1	1:A:85:LEU:HD12	1.85	0.41
1:A:345:PHE:HZ	1:B:254:ALA:HB2	1.86	0.41
1:B:27:ARG:O	1:B:31:GLU:HB3	2.21	0.41
1:A:240:ARG:HH11	1:A:276:LEU:HD23	1.86	0.41
1:B:378:LEU:O	1:B:382:GLN:HG3	2.21	0.41
1:A:15:VAL:CG1	1:A:115:ASN:HA	2.51	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	521/537 (97%)	502 (96%)	18 (4%)	1 (0%)	43	44
1	B	521/537 (97%)	501 (96%)	20 (4%)	0	100	100
All	All	1042/1074 (97%)	1003 (96%)	38 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	PRO

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	415/425 (98%)	412 (99%)	3 (1%)	76	83
1	B	415/425 (98%)	413 (100%)	2 (0%)	81	88
All	All	830/850 (98%)	825 (99%)	5 (1%)	78	86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	272	ARG
1	A	385	ARG
1	B	60	ILE
1	B	532	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	58	GLN
1	A	86	GLN
1	A	121	HIS
1	A	134	GLN
1	A	137	ASN
1	A	161	HIS
1	A	205	ASN
1	A	224	GLN
1	A	227	GLN
1	A	251	HIS
1	A	257	HIS
1	A	288	GLN
1	A	305	GLN
1	A	326	HIS
1	A	339	ASN
1	A	355	ASN
1	A	384	ASN
1	A	407	HIS
1	A	414	GLN
1	A	438	ASN
1	A	442	GLN
1	A	462	ASN

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Mol	Chain	Res	Type
1	B	115	ASN
1	B	137	ASN
1	B	161	HIS
1	B	183	GLN
1	B	205	ASN
1	B	224	GLN
1	B	251	HIS
1	B	257	HIS
1	B	280	HIS
1	B	326	HIS
1	B	407	HIS
1	B	438	ASN
1	B	442	GLN
1	B	462	ASN

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	MDO	B	152	1	11,13,14	2.59	4 (36%)	15,18,20	2.16	2 (13%)
1	MDO	A	152	2,1	11,13,14	2.60	4 (36%)	15,18,20	1.99	2 (13%)

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	MDO	B	152	1	-	2/4/23/24	0/1/1/1
1	MDO	A	152	2,1	-	2/4/23/24	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	MDO	O2-C2	6.57	1.36	1.23
1	B	152	MDO	O2-C2	6.54	1.36	1.23
1	A	152	MDO	CA2-N2	-3.24	1.33	1.39
1	B	152	MDO	CA2-N2	-3.23	1.33	1.39
1	B	152	MDO	C2-N3	-2.97	1.33	1.40
1	A	152	MDO	C2-N3	-2.94	1.33	1.40
1	A	152	MDO	C1-N3	-2.28	1.33	1.37
1	B	152	MDO	C1-N3	-2.27	1.33	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	MDO	O2-C2-CA2	-6.77	126.70	131.02
1	A	152	MDO	O2-C2-CA2	-6.08	127.14	131.02
1	B	152	MDO	CA2-C2-N3	3.57	106.50	103.50
1	A	152	MDO	CA2-C2-N3	3.41	106.36	103.50

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	152	MDO	N2-C1-CA1-CB
1	B	152	MDO	N2-C1-CA1-CB
1	A	152	MDO	N3-C1-CA1-CB
1	B	152	MDO	N3-C1-CA1-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	152	MDO	2	0
1	A	152	MDO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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
2	295	A	1001	1	14,14,14	3.08	3 (21%)	19,19,19	1.57	4 (21%)

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	295	A	1001	1	-	10/12/12/12	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	295	O1-C8	9.21	1.49	1.22
2	A	1001	295	O4-C6	5.56	1.53	1.42
2	A	1001	295	F1-C5	-2.44	1.30	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	295	O-C8-C7	4.04	124.54	113.31
2	A	1001	295	C4-C5-C	-2.74	119.21	122.80
2	A	1001	295	O1-C8-C7	-2.37	115.31	121.62
2	A	1001	295	C1-C-C5	2.04	120.48	118.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	295	C2-C6-C7-C8
2	A	1001	295	C2-C6-C7-O3
2	A	1001	295	O4-C6-C7-O3
2	A	1001	295	O3-C7-C8-O1
2	A	1001	295	O3-C7-C8-O
2	A	1001	295	C6-C7-C8-O1
2	A	1001	295	C6-C7-C8-O
2	A	1001	295	O4-C6-C7-C8
2	A	1001	295	C3-C2-C6-C7
2	A	1001	295	C1-C2-C6-C7

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	295	4	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	525/537 (97%)	-0.03	12 (2%) 61 64	12, 23, 40, 55	0
1	B	525/537 (97%)	-0.12	10 (1%) 66 69	11, 21, 41, 59	0
All	All	1050/1074 (97%)	-0.08	22 (2%) 63 66	11, 22, 41, 59	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	ALA	4.7
1	B	393	TYR	4.3
1	B	294	GLY	3.9
1	A	189	GLY	3.8
1	B	527	LEU	3.4
1	B	186	ALA	3.1
1	A	294	GLY	3.1
1	A	312	ALA	3.1
1	B	528	ARG	2.7
1	A	186	ALA	2.7
1	B	394	GLY	2.7
1	B	295	LYS	2.5
1	A	528	ARG	2.5
1	A	196	ARG	2.4
1	A	296	ASP	2.4
1	A	293	ALA	2.3
1	B	31	GLU	2.3
1	A	188	ARG	2.3
1	A	289	LYS	2.2
1	B	189	GLY	2.1
1	A	286	GLU	2.1
1	A	12	PRO	2.0

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	MDO	B	152	13/14	0.76	0.13	19,23,27,29	0
1	MDO	A	152	13/14	0.89	0.10	20,23,28,29	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
2	295	A	1001	14/14	0.36	0.27	42,44,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.