



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:39 AM UTC

PDB ID : 4O90 / pdb_00004o90
Title : Crystal structure of chorismate synthase from *Acinetobacter baumannii* at 2.6Å resolution
Authors : Chaudhary, A.; Singh, N.; Shukla, P.K.; Sinha, M.; Bhushan, A.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2013-12-31
Resolution : 2.61 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

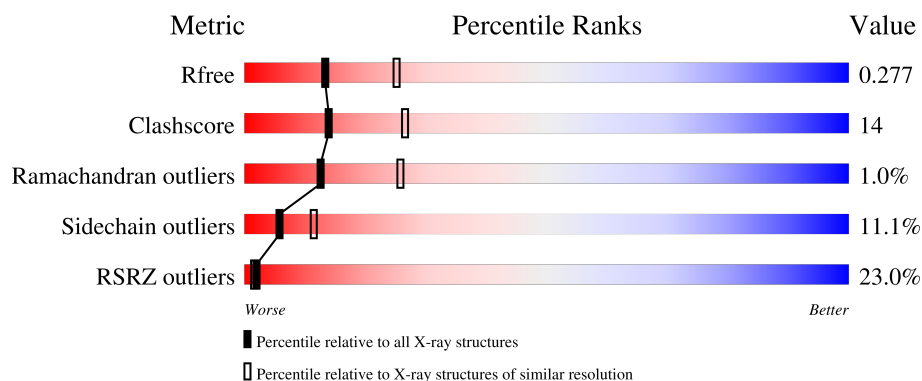
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	363	
1	B	363	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TLA	A	401	-	X	-	-
2	TLA	B	401	-	X	-	-

2 Entry composition [i](#)

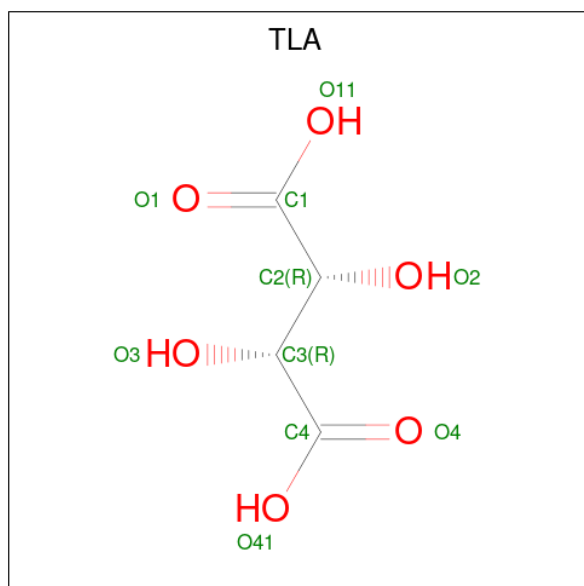
There are 4 unique types of molecules in this entry. The entry contains 4600 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2200	1376	397	416	11			
1	B	294	Total	C	N	O	S	0	0	0
			2200	1376	397	416	11			

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

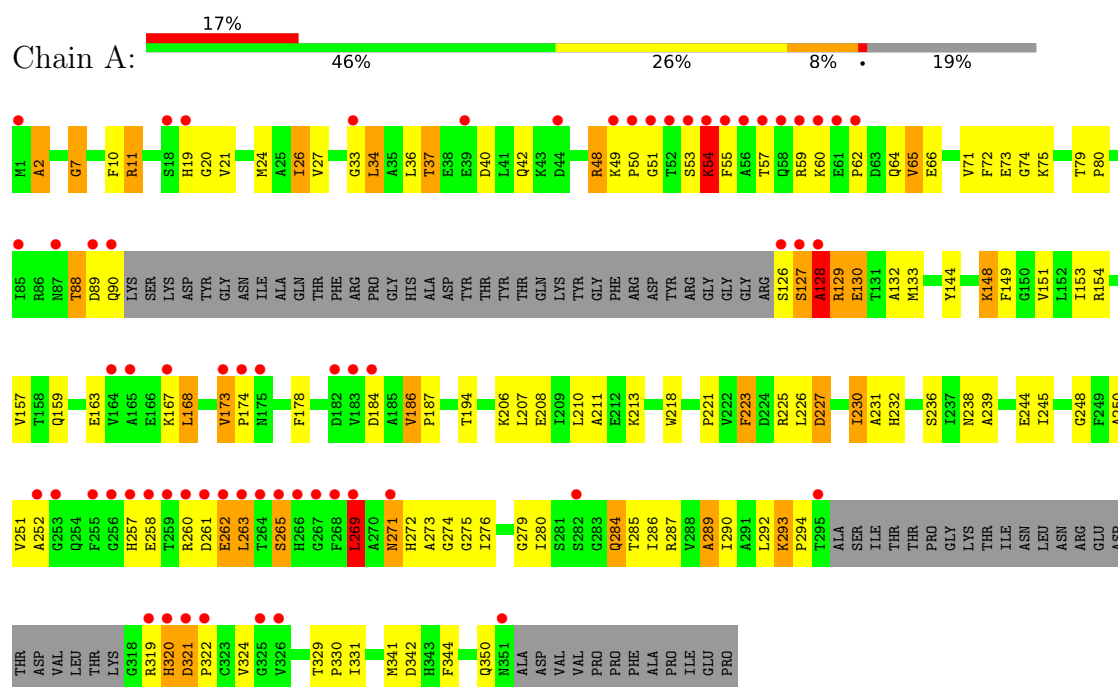
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	B	87	Total	O	0	0
			87	87		

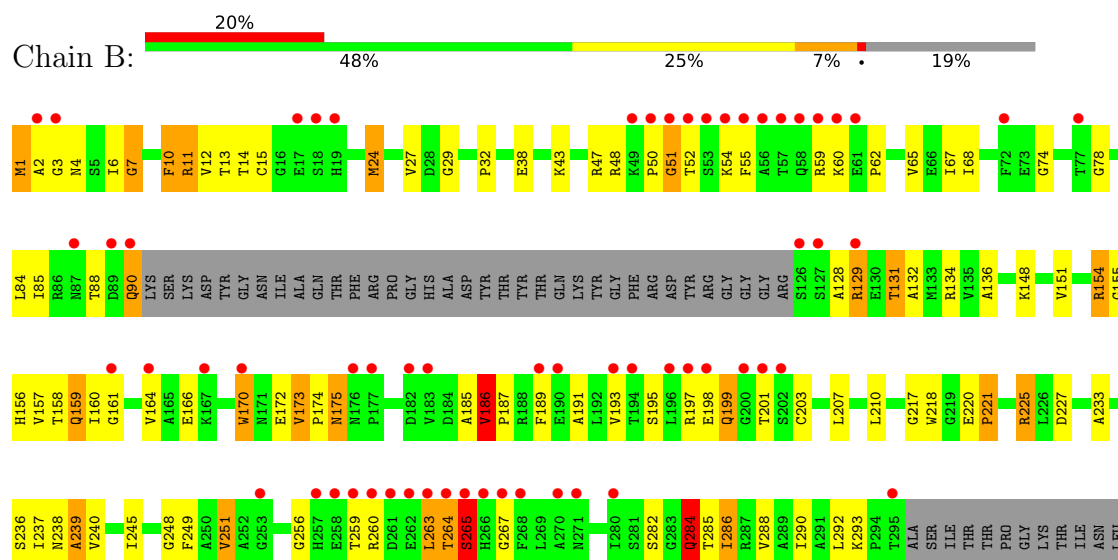
3 Residue-property plots [i](#)

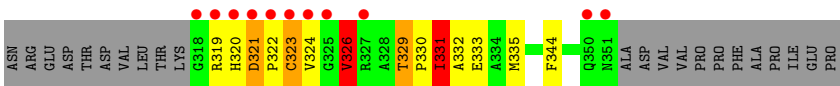
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Chorismate synthase



• Molecule 1: Chorismate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.74Å 73.19Å 90.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.37 – 2.61 32.37 – 2.61	Depositor EDS
% Data completeness (in resolution range)	93.3 (32.37-2.61) 93.2 (32.37-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.279 0.259 , 0.277	Depositor DCC
R_{free} test set	1026 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4600	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 5.75% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TLA, GOL

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	1.46	33/2236 (1.5%)	1.38	27/3021 (0.9%)
1	B	1.28	22/2236 (1.0%)	1.51	46/3021 (1.5%)
All	All	1.37	55/4472 (1.2%)	1.45	73/6042 (1.2%)

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	0	4
1	B	0	3
All	All	0	7

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173	VAL	CA-CB	11.73	1.61	1.53
1	B	329	THR	C-O	-9.33	1.15	1.24
1	B	156	HIS	CG-ND1	-8.20	1.29	1.38
1	A	36	LEU	CA-C	-7.51	1.43	1.52
1	A	280	ILE	C-O	-7.38	1.16	1.24
1	A	232	HIS	CD2-NE2	-7.21	1.29	1.37
1	A	26	ILE	C-O	-6.87	1.16	1.24
1	A	232	HIS	CG-ND1	-6.85	1.30	1.38
1	B	156	HIS	CD2-NE2	-6.85	1.30	1.37
1	A	271	ASN	CA-C	-6.66	1.45	1.53
1	A	37	THR	C-O	-6.47	1.15	1.23
1	A	257	HIS	CA-C	-6.40	1.45	1.52
1	A	252	ALA	C-O	-6.27	1.16	1.24
1	B	240	VAL	C-O	-6.26	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	THR	C-O	-6.20	1.16	1.23
1	A	173	VAL	CA-CB	6.11	1.62	1.54
1	A	36	LEU	C-O	-6.02	1.16	1.23
1	A	273	ALA	CA-C	-5.96	1.45	1.52
1	A	292	LEU	C-O	-5.94	1.16	1.23
1	A	293	LYS	C-O	-5.89	1.17	1.23
1	A	272	HIS	CG-ND1	-5.83	1.31	1.38
1	B	186	VAL	C-O	-5.81	1.19	1.24
1	A	19	HIS	CG-ND1	-5.79	1.31	1.38
1	A	232	HIS	N-CA	-5.72	1.39	1.46
1	B	332	ALA	C-O	-5.72	1.17	1.24
1	B	13	THR	C-O	-5.69	1.17	1.24
1	A	208	GLU	C-O	-5.66	1.17	1.24
1	B	156	HIS	CA-C	-5.64	1.45	1.52
1	A	290	ILE	C-O	-5.64	1.18	1.24
1	A	11	ARG	C-O	-5.56	1.17	1.23
1	B	129	ARG	C-O	-5.53	1.16	1.24
1	B	221	PRO	C-O	-5.53	1.17	1.23
1	A	21	VAL	C-O	-5.52	1.17	1.24
1	B	284	GLN	CA-C	-5.50	1.45	1.53
1	B	24	MET	C-O	-5.49	1.17	1.23
1	A	289	ALA	C-O	-5.48	1.17	1.24
1	A	27	VAL	C-O	-5.45	1.18	1.24
1	A	66	GLU	C-O	-5.45	1.17	1.24
1	B	331	ILE	C-O	-5.36	1.17	1.24
1	B	7	GLY	C-O	-5.34	1.17	1.24
1	B	285	THR	C-O	-5.29	1.17	1.23
1	A	273	ALA	C-O	-5.28	1.17	1.24
1	A	232	HIS	ND1-CE1	-5.27	1.27	1.32
1	B	286	ILE	C-O	-5.26	1.18	1.24
1	B	225	ARG	C-O	-5.26	1.17	1.23
1	B	326	VAL	C-O	-5.26	1.18	1.24
1	A	250	ALA	C-O	-5.24	1.17	1.24
1	B	151	VAL	C-O	-5.20	1.18	1.24
1	B	326	VAL	CA-CB	-5.17	1.48	1.54
1	A	231	ALA	C-O	-5.11	1.18	1.24
1	A	10	PHE	C-O	-5.09	1.17	1.24
1	A	320	HIS	CG-ND1	-5.07	1.32	1.38
1	A	223	PHE	C-O	-5.05	1.17	1.24
1	A	130	GLU	C-O	-5.04	1.17	1.24
1	B	129	ARG	CA-C	-5.01	1.45	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	THR	N-CA-C	15.93	128.72	111.36
1	B	4	ASN	N-CA-C	12.82	128.23	112.59
1	B	321	ASP	N-CA-C	-10.78	95.20	110.08
1	B	172	GLU	N-CA-C	10.28	122.56	111.36
1	A	186	VAL	CB-CA-C	-10.01	103.74	114.35
1	B	326	VAL	CB-CA-C	-8.64	100.48	112.14
1	B	132	ALA	N-CA-C	8.55	120.60	111.28
1	A	33	GLY	N-CA-C	8.34	127.66	115.32
1	B	54	LYS	N-CA-C	8.21	123.45	111.87
1	A	54	LYS	N-CA-C	7.94	121.12	109.69
1	A	127	SER	N-CA-C	7.87	120.08	108.60
1	B	199	GLN	N-CA-C	7.69	124.15	112.54
1	A	128	ALA	N-CA-C	7.37	123.17	113.30
1	A	59	ARG	N-CA-C	7.30	120.63	108.73
1	B	29	GLY	N-CA-C	7.28	124.38	114.92
1	A	262	GLU	N-CA-C	7.26	119.20	108.60
1	B	3	GLY	N-CA-C	-7.25	96.01	113.18
1	B	129	ARG	N-CA-C	-7.20	104.24	113.16
1	A	218	TRP	N-CA-C	6.99	120.87	109.76
1	A	88	THR	N-CA-C	6.96	119.99	109.41
1	A	344	PHE	N-CA-C	-6.89	103.38	111.03
1	A	236	SER	N-CA-C	-6.87	104.87	113.18
1	B	265	SER	N-CA-C	6.77	119.66	111.40
1	B	197	ARG	N-CA-C	-6.68	104.61	112.89
1	A	159	GLN	N-CA-C	6.55	119.07	108.32
1	A	130	GLU	N-CA-C	-6.55	104.87	112.92
1	A	132	ALA	N-CA-C	6.55	118.97	111.11
1	B	10	PHE	N-CA-C	-6.47	98.19	108.73
1	B	78	GLY	N-CA-C	-6.38	105.71	114.64
1	B	159	GLN	N-CA-C	6.38	118.83	108.76
1	B	55	PHE	N-CA-C	6.36	119.86	109.24
1	A	221	PRO	N-CA-C	-6.35	102.33	111.22
1	A	64	GLN	N-CA-C	6.30	118.79	108.52
1	B	217	GLY	N-CA-C	6.29	123.10	114.92
1	B	282	SER	CB-CA-C	-6.21	99.19	110.56
1	B	2	ALA	N-CA-C	6.17	119.21	110.14
1	B	158	THR	N-CA-C	-6.15	105.78	113.28
1	B	148	LYS	N-CA-C	6.11	117.74	111.14
1	B	260	ARG	CA-C-N	6.09	132.16	122.59
1	B	260	ARG	C-N-CA	6.09	132.16	122.59
1	B	170	TRP	N-CA-C	6.07	118.69	111.71
1	B	259	THR	N-CA-C	6.06	118.71	110.35
1	B	186	VAL	N-CA-C	-5.88	105.29	112.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ILE	N-CA-C	5.83	116.88	108.48
1	B	172	GLU	CA-C-N	5.83	123.91	120.24
1	B	172	GLU	C-N-CA	5.83	123.91	120.24
1	A	263	LEU	N-CA-C	-5.78	106.46	112.93
1	A	265	SER	N-CA-C	5.72	116.84	108.14
1	B	136	ALA	N-CA-C	-5.71	105.05	111.28
1	B	164	VAL	N-CA-C	5.69	116.08	108.11
1	A	19	HIS	CB-CA-C	5.68	120.16	111.02
1	A	320	HIS	N-CA-C	5.65	118.30	108.76
1	B	154	ARG	N-CA-C	5.63	117.83	108.99
1	B	236	SER	N-CA-C	-5.60	106.44	113.28
1	B	332	ALA	N-CA-C	-5.59	105.18	111.28
1	B	288	VAL	CB-CA-C	-5.53	101.99	110.50
1	B	62	PRO	N-CA-C	5.49	123.78	112.47
1	B	267	GLY	N-CA-C	5.49	126.19	113.18
1	B	221	PRO	CA-C-O	-5.28	115.32	122.08
1	A	60	LYS	N-CA-C	5.28	117.34	110.53
1	B	239	ALA	N-CA-CB	-5.26	108.84	114.10
1	B	4	ASN	N-CA-CB	-5.26	102.51	110.92
1	B	14	THR	N-CA-C	5.23	117.36	109.41
1	A	148	LYS	N-CA-C	5.20	116.76	111.14
1	B	263	LEU	N-CA-C	5.20	121.86	110.80
1	A	71	VAL	N-CA-C	5.15	115.69	108.17
1	B	74	GLY	N-CA-C	5.06	122.10	115.47
1	A	168	LEU	N-CA-C	5.04	116.63	108.41
1	A	65	VAL	N-CA-C	5.03	115.59	109.30
1	B	32	PRO	N-CA-C	-5.03	103.93	111.57
1	B	285	THR	N-CA-C	-5.03	103.51	110.35
1	A	7	GLY	CA-C-O	-5.02	118.77	122.23
1	B	233	ALA	N-CA-C	5.01	116.43	111.07

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ALA	Peptide
1	A	2	ALA	Peptide
1	A	269	LEU	Peptide
1	A	53	SER	Peptide
1	B	256	GLY	Peptide
1	B	265	SER	Peptide
1	B	321	ASP	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	2200	0	2203	63	0
1	B	2200	0	2203	68	0
2	A	10	0	4	2	0
2	B	10	0	4	1	0
3	A	6	0	8	0	0
3	B	6	0	8	2	0
4	A	81	0	0	2	0
4	B	87	0	0	5	0
All	All	4600	0	4430	128	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 14.

All (128) 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:225:ARG:HG2	1:A:279:GLY:HA3	1.44	0.97
1:B:90:GLN:HA	1:B:90:GLN:OE1	1.74	0.87
1:B:237:ILE:HG12	1:B:331:ILE:HD11	1.62	0.82
1:A:51:GLY:CA	1:A:54:LYS:HB3	2.10	0.82
1:A:49:LYS:O	1:A:49:LYS:HG3	1.79	0.81
1:B:186:VAL:HB	1:B:187:PRO:HD3	1.62	0.80
1:A:48:ARG:O	1:A:50:PRO:HD3	1.82	0.79
1:A:271:ASN:HD21	1:A:284:GLN:HB2	1.48	0.78
1:B:90:GLN:OE1	1:B:90:GLN:CA	2.30	0.78
1:B:238:ASN:O	1:B:239:ALA:HB3	1.82	0.77
1:B:290:ILE:HD12	1:B:292:LEU:HD11	1.69	0.74
1:B:237:ILE:HG12	1:B:331:ILE:CD1	2.19	0.73
1:A:51:GLY:HA2	1:A:54:LYS:HB3	1.70	0.73
1:A:20:GLY:HA3	4:A:517:HOH:O	1.89	0.73
1:A:293:LYS:HA	1:B:251:VAL:HG13	1.69	0.72
1:B:323:CYS:O	1:B:326:VAL:HG22	1.92	0.69
1:B:323:CYS:O	1:B:326:VAL:CG2	2.41	0.68
1:B:237:ILE:CG1	1:B:331:ILE:HD11	2.24	0.67
1:A:184:ASP:O	1:A:187:PRO:HG2	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PHE:HB3	1:B:6:ILE:HD13	1.79	0.64
1:B:238:ASN:O	1:B:239:ALA:CB	2.45	0.63
1:B:186:VAL:N	1:B:187:PRO:CD	2.59	0.63
1:B:38:GLU:HG3	1:B:67:ILE:HG13	1.80	0.63
1:A:211:ALA:HB3	1:A:286:ILE:HB	1.81	0.62
1:A:49:LYS:O	1:A:49:LYS:CG	2.47	0.62
1:B:186:VAL:CB	1:B:187:PRO:HD3	2.30	0.61
1:B:290:ILE:CD1	1:B:292:LEU:HD11	2.31	0.61
1:A:65:VAL:HG13	1:A:65:VAL:O	1.99	0.61
1:A:51:GLY:HA3	1:A:54:LYS:HB3	1.83	0.60
1:A:321:ASP:HB3	1:A:324:VAL:HB	1.84	0.60
1:B:329:THR:HB	1:B:330:PRO:HD3	1.84	0.60
1:A:51:GLY:HA2	1:A:54:LYS:CB	2.31	0.59
1:A:226:LEU:O	1:A:230:ILE:HG12	2.03	0.58
1:A:127:SER:C	1:A:129:ARG:HB2	2.29	0.58
1:B:248:GLY:O	1:B:251:VAL:HB	2.02	0.58
1:A:238:ASN:O	1:A:239:ALA:HB3	2.04	0.57
1:A:261:ASP:HA	4:A:573:HOH:O	2.04	0.57
1:B:48:ARG:NH1	1:B:128:ALA:O	2.37	0.57
1:B:160:ILE:CG2	1:B:203:CYS:SG	2.95	0.54
1:B:134:ARG:HG2	1:B:335:MET:HE1	1.90	0.54
1:A:293:LYS:HB2	1:A:294:PRO:HD2	1.90	0.54
1:A:227:ASP:OD1	1:A:227:ASP:N	2.36	0.54
2:A:401:TLA:O11	2:A:401:TLA:O3	2.23	0.52
1:B:186:VAL:N	1:B:187:PRO:HD2	2.24	0.52
1:A:275:GLY:C	1:A:276:ILE:HG13	2.34	0.52
1:B:175:ASN:OD1	1:B:175:ASN:N	2.36	0.52
1:B:157:VAL:HG21	1:B:326:VAL:HG12	1.91	0.52
1:B:15:CYS:SG	1:B:24:MET:HB2	2.50	0.51
1:B:160:ILE:HG22	1:B:203:CYS:SG	2.49	0.51
1:B:319:ARG:HD2	4:B:563:HOH:O	2.11	0.51
1:B:160:ILE:O	1:B:161:GLY:C	2.51	0.51
1:B:237:ILE:HG12	1:B:331:ILE:CG1	2.41	0.51
1:A:48:ARG:C	1:A:50:PRO:HD3	2.36	0.51
1:A:350:GLN:HG3	1:B:1:MET:HE2	1.93	0.51
1:B:186:VAL:O	1:B:189:PHE:HB2	2.11	0.50
1:A:24:MET:HA	1:A:133:MET:HE3	1.93	0.49
1:A:34:LEU:HD13	1:A:144:TYR:HA	1.94	0.49
1:A:319:ARG:C	1:A:320:HIS:CD2	2.90	0.49
1:A:271:ASN:ND2	1:A:284:GLN:HB2	2.24	0.49
2:A:401:TLA:O4	2:A:401:TLA:O2	2.31	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:TLA:H2	3:B:402:GOL:H11	1.95	0.49
1:A:128:ALA:N	1:A:129:ARG:HB2	2.28	0.48
1:B:68:ILE:HD11	1:B:84:LEU:HB3	1.96	0.48
1:B:159:GLN:OE1	3:B:402:GOL:H2	2.14	0.48
1:B:173:VAL:HG22	1:B:174:PRO:HD3	1.95	0.48
1:B:50:PRO:O	1:B:51:GLY:O	2.32	0.48
1:A:293:LYS:HB2	1:A:294:PRO:CD	2.44	0.48
1:B:220:GLU:HA	1:B:221:PRO:HD2	1.77	0.47
1:B:155:GLY:N	1:B:333:GLU:OE2	2.45	0.47
1:A:244:GLU:HB2	1:A:248:GLY:HA3	1.96	0.47
1:A:24:MET:CA	1:A:133:MET:HE3	2.45	0.47
1:A:274:GLY:O	1:A:286:ILE:HA	2.15	0.47
1:B:7:GLY:HA3	1:B:10:PHE:O	2.15	0.47
1:A:7:GLY:O	1:A:11:ARG:HG3	2.15	0.46
1:A:79:THR:O	1:A:80:PRO:C	2.58	0.46
1:A:210:LEU:HD21	1:A:287:ARG:HG3	1.97	0.46
1:A:72:PHE:O	1:A:73:GLU:C	2.56	0.46
1:A:248:GLY:O	1:A:251:VAL:HG22	2.15	0.46
1:A:238:ASN:O	1:A:239:ALA:CB	2.63	0.46
1:A:244:GLU:HG2	1:A:289:ALA:HB3	1.98	0.46
1:B:48:ARG:HH11	1:B:131:THR:HG22	1.81	0.46
1:A:51:GLY:CA	1:A:54:LYS:CB	2.89	0.46
1:A:74:GLY:C	1:A:75:LYS:HG2	2.40	0.45
1:B:237:ILE:HG12	1:B:331:ILE:HG12	1.98	0.45
1:A:173:VAL:HG22	1:A:174:PRO:HD3	1.98	0.45
1:B:326:VAL:HG22	1:B:326:VAL:H	1.43	0.45
1:A:89:ASP:OD2	1:A:90:GLN:NE2	2.50	0.45
1:A:329:THR:HB	1:A:330:PRO:HD3	1.99	0.45
1:B:60:LYS:HA	4:B:504:HOH:O	2.17	0.44
1:A:42:GLN:OE1	1:A:65:VAL:HG12	2.17	0.44
1:B:90:GLN:OE1	1:B:90:GLN:N	2.50	0.44
1:B:65:VAL:HA	1:B:85:ILE:HG12	1.99	0.44
1:B:191:ALA:O	1:B:195:SER:HB2	2.18	0.44
1:A:153:ILE:HA	1:A:210:LEU:O	2.18	0.43
1:A:350:GLN:HG3	1:B:1:MET:CE	2.48	0.43
1:B:284:GLN:H	1:B:284:GLN:HG2	1.47	0.43
1:A:167:LYS:HG2	1:A:168:LEU:N	2.33	0.43
1:B:166:GLU:HB3	4:B:532:HOH:O	2.18	0.43
1:B:284:GLN:HB3	4:B:544:HOH:O	2.19	0.43
1:B:68:ILE:HD12	1:B:68:ILE:N	2.33	0.43
1:A:2:ALA:HA	1:B:221:PRO:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ILE:O	1:B:335:MET:HG2	2.19	0.43
1:A:269:LEU:N	1:A:269:LEU:HD23	2.34	0.42
1:A:319:ARG:HG3	1:A:319:ARG:HH11	1.84	0.42
1:B:170:TRP:HZ2	1:B:210:LEU:HD12	1.84	0.42
1:A:350:GLN:CG	1:B:1:MET:HE2	2.49	0.42
1:B:6:ILE:HG22	1:B:12:VAL:HB	2.00	0.42
1:A:210:LEU:CD2	1:A:287:ARG:HG3	2.49	0.42
1:A:37:THR:HG22	1:A:40:ASP:OD2	2.20	0.42
1:B:6:ILE:O	1:B:11:ARG:HA	2.20	0.42
1:B:51:GLY:HA3	1:B:52:THR:HA	1.72	0.42
1:A:151:VAL:HG23	1:A:213:LYS:O	2.19	0.41
1:B:131:THR:O	1:B:131:THR:HG23	2.19	0.41
1:B:225:ARG:HB3	1:B:227:ASP:OD1	2.20	0.41
1:B:218:TRP:CH2	1:B:344:PHE:HB2	2.55	0.41
1:A:148:LYS:HG2	1:A:149:PHE:CE2	2.56	0.41
1:B:249:PHE:C	1:B:251:VAL:H	2.28	0.41
1:B:207:LEU:HD13	1:B:292:LEU:HD13	2.03	0.41
1:A:128:ALA:O	1:A:130:GLU:HG2	2.21	0.41
1:A:271:ASN:HD21	1:A:284:GLN:CB	2.24	0.41
1:B:11:ARG:O	1:B:27:VAL:HA	2.20	0.41
1:B:47:ARG:O	1:B:50:PRO:HD3	2.19	0.41
1:B:185:ALA:O	1:B:186:VAL:C	2.61	0.41
1:A:207:LEU:O	1:A:289:ALA:HA	2.21	0.41
1:A:341:MET:O	1:A:342:ASP:C	2.64	0.41
1:B:38:GLU:HB2	4:B:514:HOH:O	2.20	0.40
1:B:210:LEU:HA	1:B:286:ILE:O	2.21	0.40
1:A:157:VAL:HG21	1:A:178:PHE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	288/363 (79%)	273 (95%)	12 (4%)	3 (1%)	12	26
1	B	288/363 (79%)	271 (94%)	14 (5%)	3 (1%)	12	26
All	All	576/726 (79%)	544 (94%)	26 (4%)	6 (1%)	12	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	GLY
1	B	322	PRO
1	B	263	LEU
1	A	322	PRO
1	A	55	PHE
1	A	62	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	229/286 (80%)	204 (89%)	25 (11%)	6	12
1	B	229/286 (80%)	203 (89%)	26 (11%)	5	10
All	All	458/572 (80%)	407 (89%)	51 (11%)	6	11

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	34	LEU
1	A	48	ARG
1	A	54	LYS
1	A	57	THR
1	A	88	THR
1	A	126	SER
1	A	129	ARG
1	A	154	ARG
1	A	163	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	186	VAL
1	A	194	THR
1	A	206	LYS
1	A	227	ASP
1	A	230	ILE
1	A	245	ILE
1	A	258	GLU
1	A	260	ARG
1	A	262	GLU
1	A	263	LEU
1	A	265	SER
1	A	269	LEU
1	A	284	GLN
1	A	321	ASP
1	A	331	ILE
1	B	1	MET
1	B	11	ARG
1	B	43	LYS
1	B	59	ARG
1	B	88	THR
1	B	90	GLN
1	B	129	ARG
1	B	131	THR
1	B	154	ARG
1	B	175	ASN
1	B	186	VAL
1	B	193	VAL
1	B	198	GLU
1	B	199	GLN
1	B	201	THR
1	B	245	ILE
1	B	251	VAL
1	B	264	THR
1	B	265	SER
1	B	284	GLN
1	B	293	LYS
1	B	320	HIS
1	B	323	CYS
1	B	324	VAL
1	B	326	VAL
1	B	331	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	90	GLN
1	A	171	ASN
1	A	199	GLN
1	A	320	HIS
1	B	266	HIS

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 ⓘ

4 ligands 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	$\# Z > 2$
2	TLA	B	401	-	9,9,9	2.61	5 (55%)	12,12,12	1.16	2 (16%)
3	GOL	B	402	-	5,5,5	0.56	0	5,5,5	0.34	0
2	TLA	A	401	-	9,9,9	3.28	6 (66%)	12,12,12	1.83	5 (41%)
3	GOL	A	402	-	5,5,5	0.40	0	5,5,5	0.23	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	TLA	B	401	-	-	11/12/12/12	-
3	GOL	B	402	-	-	3/4/4/4	-
2	TLA	A	401	-	-	10/12/12/12	-
3	GOL	A	402	-	-	0/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	TLA	C3-C4	6.54	1.62	1.52
2	B	401	TLA	O1-C1	4.66	1.35	1.22
2	B	401	TLA	O11-C1	-4.04	1.17	1.30
2	A	401	TLA	O4-C4	-4.02	1.10	1.22
2	A	401	TLA	O2-C2	3.75	1.49	1.42
2	A	401	TLA	C3-C2	-2.95	1.44	1.53
2	B	401	TLA	O41-C4	-2.58	1.22	1.30
2	B	401	TLA	C2-C1	-2.56	1.49	1.52
2	B	401	TLA	O4-C4	2.52	1.29	1.22
2	A	401	TLA	C2-C1	2.39	1.56	1.52
2	A	401	TLA	O11-C1	-2.05	1.24	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	TLA	O1-C1-C2	-2.62	114.65	121.62
2	A	401	TLA	O3-C3-C4	-2.49	105.36	110.69
2	B	401	TLA	O11-C1-C2	2.46	120.15	113.31
2	A	401	TLA	O2-C2-C1	-2.40	105.55	110.69
2	A	401	TLA	O2-C2-C3	2.23	114.69	110.17
2	B	401	TLA	O1-C1-C2	-2.17	115.83	121.62
2	A	401	TLA	O41-C4-O4	2.08	128.81	124.08

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	TLA	C1-C2-C3-C4
2	A	401	TLA	O2-C2-C3-O3
2	B	401	TLA	O1-C1-C2-O2
2	B	401	TLA	O11-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	402	GOL	C1-C2-C3-O3
2	A	401	TLA	O3-C3-C4-O41
2	B	401	TLA	O3-C3-C4-O4
2	B	401	TLA	O3-C3-C4-O41
2	A	401	TLA	O1-C1-C2-C3
2	A	401	TLA	C2-C3-C4-O4
2	A	401	TLA	C2-C3-C4-O41
2	B	401	TLA	O11-C1-C2-C3
2	A	401	TLA	C1-C2-C3-O3
2	A	401	TLA	O2-C2-C3-C4
2	A	401	TLA	O3-C3-C4-O4
2	B	401	TLA	O1-C1-C2-C3
3	B	402	GOL	O2-C2-C3-O3
2	A	401	TLA	O1-C1-C2-O2
2	B	401	TLA	C2-C3-C4-O41
2	B	401	TLA	C1-C2-C3-O3
3	B	402	GOL	O1-C1-C2-O2
2	B	401	TLA	O2-C2-C3-O3
2	B	401	TLA	C2-C3-C4-O4
2	B	401	TLA	O2-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	TLA	1	0
3	B	402	GOL	2	0
2	A	401	TLA	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	294/363 (80%)	1.70	63 (21%) 2 2	5, 28, 61, 99	22 (7%)
1	B	294/363 (80%)	1.98	72 (24%) 2 1	5, 30, 77, 100	22 (7%)
All	All	588/726 (80%)	1.84	135 (22%) 2 1	5, 29, 70, 100	44 (7%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	PHE	19.9
1	A	55	PHE	17.3
1	A	268	PHE	16.3
1	A	263	LEU	15.3
1	B	56	ALA	15.0
1	A	61	GLU	14.9
1	B	57	THR	14.8
1	B	268	PHE	14.5
1	A	267	GLY	14.0
1	B	267	GLY	14.0
1	A	54	LYS	13.5
1	A	257	HIS	13.5
1	B	257	HIS	13.4
1	A	266	HIS	13.2
1	A	264	THR	13.0
1	A	52	THR	13.0
1	A	57	THR	12.7
1	A	53	SER	12.5
1	B	264	THR	12.5
1	B	266	HIS	12.4
1	B	263	LEU	12.4
1	B	259	THR	12.4
1	B	61	GLU	12.2
1	B	260	ARG	12.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	52	THR	12.1
1	B	54	LYS	12.1
1	A	60	LYS	12.0
1	B	60	LYS	11.7
1	A	258	GLU	11.5
1	B	258	GLU	11.5
1	A	56	ALA	10.6
1	B	58	GLN	10.0
1	B	265	SER	9.9
1	A	259	THR	9.5
1	B	53	SER	9.2
1	B	261	ASP	9.2
1	A	59	ARG	9.1
1	A	260	ARG	9.0
1	B	262	GLU	8.8
1	B	59	ARG	8.5
1	A	262	GLU	7.5
1	A	58	GLN	7.2
1	A	261	ASP	7.1
1	B	321	ASP	7.1
1	A	265	SER	6.7
1	B	51	GLY	5.8
1	B	198	GLU	4.9
1	A	49	LYS	4.6
1	A	50	PRO	4.5
1	A	184	ASP	4.5
1	B	49	LYS	4.4
1	B	126	SER	4.4
1	A	127	SER	4.4
1	B	167	LYS	4.3
1	B	183	VAL	4.3
1	A	253	GLY	4.2
1	B	327	ARG	4.1
1	A	128	ALA	3.9
1	A	326	VAL	3.9
1	B	190	GLU	3.8
1	B	197	ARG	3.8
1	B	50	PRO	3.7
1	B	318	GLY	3.7
1	B	200	GLY	3.6
1	A	167	LYS	3.5
1	A	126	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	127	SER	3.4
1	A	256	GLY	3.4
1	B	161	GLY	3.4
1	B	194	THR	3.3
1	A	319	ARG	3.2
1	B	3	GLY	3.2
1	A	19	HIS	3.1
1	B	164	VAL	3.1
1	B	201	THR	3.0
1	A	321	ASP	3.0
1	B	89	ASP	3.0
1	A	295	THR	3.0
1	B	323	CYS	2.9
1	A	183	VAL	2.9
1	B	320	HIS	2.9
1	A	182	ASP	2.9
1	B	90	GLN	2.9
1	B	324	VAL	2.9
1	B	193	VAL	2.8
1	B	351	ASN	2.8
1	B	325	GLY	2.8
1	A	165	ALA	2.8
1	B	270	ALA	2.8
1	A	90	GLN	2.7
1	B	87	ASN	2.7
1	B	18	SER	2.7
1	A	89	ASP	2.7
1	B	295	THR	2.7
1	A	33	GLY	2.7
1	A	351	ASN	2.6
1	B	2	ALA	2.6
1	A	271	ASN	2.6
1	B	176	ASN	2.6
1	B	319	ARG	2.5
1	A	87	ASN	2.5
1	A	255	PHE	2.5
1	A	320	HIS	2.4
1	B	189	PHE	2.4
1	B	196	LEU	2.3
1	B	202	SER	2.3
1	A	269	LEU	2.3
1	B	77	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	164	VAL	2.3
1	A	39	GLU	2.2
1	A	282	SER	2.2
1	A	173	VAL	2.2
1	B	177	PRO	2.2
1	A	51	GLY	2.2
1	A	18	SER	2.2
1	B	129	ARG	2.2
1	A	174	PRO	2.1
1	B	322	PRO	2.1
1	A	175	ASN	2.1
1	A	85	ILE	2.1
1	B	19	HIS	2.1
1	B	170	TRP	2.1
1	A	1	MET	2.1
1	B	350	GLN	2.1
1	B	253	GLY	2.1
1	A	62	PRO	2.1
1	A	322	PRO	2.1
1	A	325	GLY	2.1
1	B	72	PHE	2.1
1	A	252	ALA	2.0
1	B	280	ILE	2.0
1	A	44	ASP	2.0
1	B	17	GLU	2.0
1	B	182	ASP	2.0
1	B	271	ASN	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	TLA	B	401	10/10	0.56	0.25	89,90,91,93	0
2	TLA	A	401	10/10	0.58	0.20	80,81,81,81	0
3	GOL	A	402	6/6	0.61	0.24	77,77,78,78	0
3	GOL	B	402	6/6	0.61	0.24	64,73,75,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.