



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:58 AM UTC

PDB ID : 1WSZ / pdb_00001wsz
Title : Mutant human ABO(H) blood group transferase A
Authors : Lee, H.J.; Barry, C.H.; Borisova, S.N.; Seto, N.O.L.; Zheng, R.B.; Blancher, A.; Evans, S.V.; Palcic, M.M.
Deposited on : 2004-11-12
Resolution : 1.59 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
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

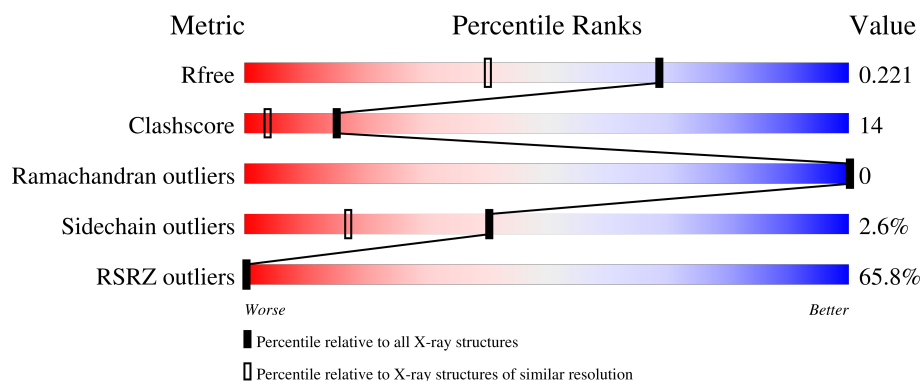
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	292	59% 70% 18% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2365 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 Histo-blood group ABO system transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2145	1394	366	375	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	initiating methionine	UNP P16442
A	74	SER	PRO	engineered mutation	UNP P16442

- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Hg	0	0
			4	4		

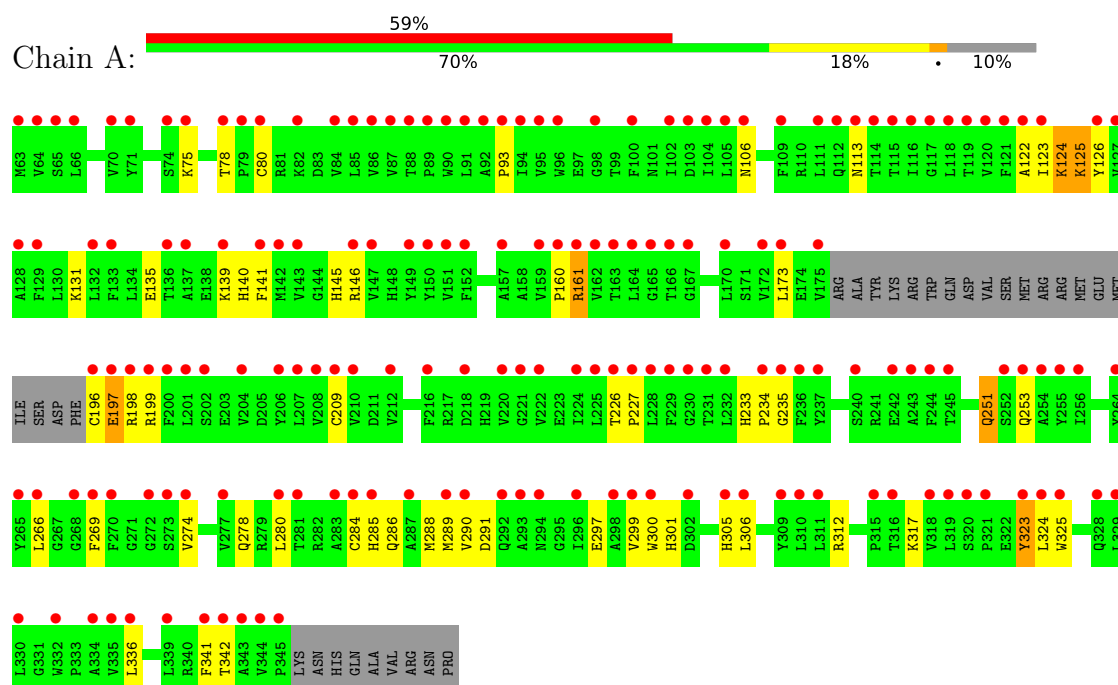
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	216	Total	O	0	0
			216	216		

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: Histo-blood group ABO system transferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	52.70Å 150.10Å 79.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.59 20.00 – 1.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.59) 98.6 (20.00-1.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 1.59Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.209 , 0.244 0.201 , 0.221	Depositor DCC
R_{free} test set	261 reflections (0.61%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 42.3	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	0.95	EDS
Total number of atoms	2365	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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: HG

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	0.36	0/2205	0.89	4/2997 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	LYS	CB-CA-C	-5.63	110.09	116.63
1	A	342	THR	N-CA-C	5.53	117.60	109.24
1	A	323	TYR	N-CA-C	5.12	119.38	113.18
1	A	141	PHE	N-CA-C	5.05	116.55	108.41

There are no chirality outliers.

There are no planarity outliers.

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	2145	0	2130	58	0
2	A	4	0	0	0	0
3	A	216	0	0	2	0
All	All	2365	0	2130	58	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 (58) 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:125:LYS:HD3	1:A:125:LYS:H	1.24	1.01
1:A:161:ARG:NE	1:A:161:ARG:HA	1.82	0.93
1:A:123:ILE:HG22	1:A:124:LYS:HG3	1.57	0.84
1:A:233:HIS:HD2	1:A:235:GLY:H	1.24	0.83
1:A:266:LEU:HD13	1:A:324:LEU:HD13	1.65	0.77
1:A:125:LYS:HD3	1:A:125:LYS:N	1.99	0.75
1:A:139:LYS:O	1:A:139:LYS:HD3	1.86	0.74
1:A:226:THR:HG21	1:A:317:LYS:HB2	1.69	0.74
1:A:251:GLN:NE2	1:A:251:GLN:H	1.86	0.73
1:A:196:CYS:HA	1:A:198:ARG:NH1	2.06	0.71
1:A:196:CYS:HB2	1:A:199:ARG:NH2	2.06	0.71
1:A:125:LYS:H	1:A:125:LYS:CD	2.03	0.69
1:A:199:ARG:NH1	1:A:199:ARG:HB3	2.12	0.64
1:A:233:HIS:CD2	1:A:235:GLY:H	2.13	0.64
1:A:285:HIS:O	1:A:289:MET:HG3	1.98	0.64
1:A:139:LYS:HD2	1:A:140:HIS:NE2	2.14	0.63
1:A:274:VAL:O	1:A:278:GLN:HG3	2.00	0.61
1:A:251:GLN:H	1:A:251:GLN:HE21	1.49	0.60
1:A:75:LYS:HB2	1:A:78:THR:HB	1.84	0.59
1:A:233:HIS:HA	1:A:266:LEU:HG	1.83	0.59
1:A:325:TRP:CZ3	1:A:336:LEU:HD11	2.38	0.59
1:A:139:LYS:HD2	1:A:140:HIS:CE1	2.39	0.58
1:A:123:ILE:CG2	1:A:124:LYS:HG3	2.32	0.57
1:A:93:PRO:HG2	1:A:317:LYS:HG2	1.89	0.55
1:A:284:CYS:O	1:A:288:MET:HG3	2.07	0.54
1:A:113:ASN:HD21	1:A:146:ARG:HH11	1.55	0.54
1:A:122:ALA:C	1:A:123:ILE:HD12	2.33	0.54
1:A:269:PHE:HB2	1:A:324:LEU:HD12	1.91	0.53
1:A:196:CYS:HA	1:A:198:ARG:HH12	1.73	0.53
1:A:197:GLU:H	1:A:197:GLU:CD	2.17	0.53
1:A:139:LYS:HD3	1:A:139:LYS:C	2.34	0.53
1:A:280:LEU:C	1:A:280:LEU:HD23	2.33	0.53
1:A:323:TYR:O	1:A:341:PHE:HB3	2.08	0.53
1:A:234:PRO:HD3	1:A:266:LEU:HD11	1.92	0.51
1:A:106:ASN:OD1	1:A:145:HIS:HE1	1.96	0.48
1:A:125:LYS:HE2	1:A:126:TYR:CE1	2.49	0.48
1:A:197:GLU:HB3	1:A:278:GLN:NE2	2.29	0.47
1:A:305:HIS:HE1	3:A:552:HOH:O	1.97	0.47
1:A:286:GLN:O	1:A:290:VAL:HG23	2.15	0.47
1:A:113:ASN:ND2	1:A:146:ARG:HH11	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PRO:HG3	3:A:712:HOH:O	2.15	0.46
1:A:306:LEU:C	1:A:306:LEU:HD23	2.41	0.46
1:A:199:ARG:HB3	1:A:199:ARG:HH11	1.79	0.46
1:A:161:ARG:HA	1:A:161:ARG:HE	1.76	0.46
1:A:226:THR:HG1	1:A:227:PRO:HD2	1.80	0.45
1:A:197:GLU:N	1:A:197:GLU:OE1	2.49	0.45
1:A:325:TRP:CE3	1:A:336:LEU:HD11	2.52	0.44
1:A:325:TRP:CH2	1:A:336:LEU:HD11	2.52	0.44
1:A:251:GLN:NE2	1:A:251:GLN:N	2.61	0.44
1:A:123:ILE:HD12	1:A:123:ILE:N	2.33	0.43
1:A:131:LYS:O	1:A:135:GLU:HG3	2.18	0.43
1:A:299:VAL:HG13	1:A:300:TRP:N	2.34	0.43
1:A:312:ARG:HD3	1:A:312:ARG:HA	1.74	0.42
1:A:113:ASN:HD21	1:A:146:ARG:NH1	2.17	0.42
1:A:173:LEU:HD22	1:A:173:LEU:N	2.34	0.42
1:A:288:MET:HG2	1:A:305:HIS:CE1	2.53	0.42
1:A:297:GLU:OE2	1:A:301:HIS:HD2	2.03	0.41
1:A:253:GLN:HG2	1:A:291:ASP:OD1	2.21	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	259/292 (89%)	252 (97%)	7 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	233/260 (90%)	227 (97%)	6 (3%)	40 17

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	CYS
1	A	125	LYS
1	A	161	ARG
1	A	197	GLU
1	A	209	CYS
1	A	251	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	113	ASN
1	A	145	HIS
1	A	155	GLN
1	A	169	GLN
1	A	233	HIS
1	A	251	GLN
1	A	278	GLN
1	A	285	HIS
1	A	286	GLN
1	A	301	HIS
1	A	305	HIS
1	A	313	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	263/292 (90%)	2.36	173 (65%) 0 0	15, 24, 39, 56	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	CYS	9.0
1	A	197	GLU	4.9
1	A	198	ARG	4.8
1	A	266	LEU	4.8
1	A	63	MET	4.7
1	A	196	CYS	4.5
1	A	293	ALA	4.4
1	A	161	ARG	4.3
1	A	121	PHE	4.3
1	A	95	VAL	3.9
1	A	175	VAL	3.9
1	A	299	VAL	3.9
1	A	201	LEU	3.9
1	A	335	VAL	3.8
1	A	92	ALA	3.7
1	A	94	ILE	3.7
1	A	172	VAL	3.6
1	A	220	VAL	3.6
1	A	90	TRP	3.5
1	A	79	PRO	3.5
1	A	325	TRP	3.5
1	A	209	CYS	3.5
1	A	139	LYS	3.5
1	A	284	CYS	3.4
1	A	147	VAL	3.4
1	A	345	PRO	3.4
1	A	228	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	123	ILE	3.3
1	A	280	LEU	3.3
1	A	64	VAL	3.3
1	A	96	TRP	3.3
1	A	199	ARG	3.3
1	A	87	VAL	3.3
1	A	82	LYS	3.2
1	A	226	THR	3.2
1	A	120	VAL	3.2
1	A	143	VAL	3.2
1	A	298	ALA	3.2
1	A	316	THR	3.1
1	A	344	VAL	3.1
1	A	283	ALA	3.1
1	A	224	ILE	3.1
1	A	277	VAL	3.1
1	A	113	ASN	3.1
1	A	339	LEU	3.1
1	A	216	PHE	3.1
1	A	229	PHE	3.1
1	A	137	ALA	3.1
1	A	222	VAL	3.0
1	A	306	LEU	3.0
1	A	270	PHE	3.0
1	A	112	GLN	3.0
1	A	105	LEU	3.0
1	A	300	TRP	3.0
1	A	85	LEU	3.0
1	A	225	LEU	3.0
1	A	272	GLY	2.9
1	A	88	THR	2.9
1	A	227	PRO	2.9
1	A	146	ARG	2.9
1	A	126	TYR	2.9
1	A	281	THR	2.9
1	A	319	LEU	2.9
1	A	336	LEU	2.9
1	A	302	ASP	2.8
1	A	84	VAL	2.8
1	A	329	LEU	2.8
1	A	152	PHE	2.8
1	A	116	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	86	VAL	2.8
1	A	127	VAL	2.8
1	A	159	VAL	2.8
1	A	102	ILE	2.8
1	A	256	ILE	2.8
1	A	309	TYR	2.8
1	A	207	LEU	2.8
1	A	274	VAL	2.7
1	A	114	THR	2.7
1	A	119	THR	2.7
1	A	236	PHE	2.7
1	A	318	VAL	2.7
1	A	109	PHE	2.7
1	A	244	PHE	2.7
1	A	162	VAL	2.7
1	A	290	VAL	2.7
1	A	78	THR	2.7
1	A	269	PHE	2.6
1	A	323	TYR	2.6
1	A	132	LEU	2.6
1	A	75	LYS	2.6
1	A	315	PRO	2.6
1	A	104	ILE	2.6
1	A	264	TYR	2.6
1	A	265	TYR	2.6
1	A	208	VAL	2.6
1	A	212	VAL	2.6
1	A	89	PRO	2.6
1	A	129	PHE	2.5
1	A	133	PHE	2.5
1	A	200	PHE	2.5
1	A	206	TYR	2.5
1	A	341	PHE	2.5
1	A	321	PRO	2.5
1	A	254	ALA	2.5
1	A	296	ILE	2.5
1	A	255	TYR	2.5
1	A	310	LEU	2.5
1	A	330	LEU	2.5
1	A	289	MET	2.5
1	A	100	PHE	2.5
1	A	141	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	70	VAL	2.5
1	A	210	VAL	2.5
1	A	65	SER	2.4
1	A	221	GLY	2.4
1	A	230	GLY	2.4
1	A	118	LEU	2.4
1	A	157	ALA	2.4
1	A	202	SER	2.4
1	A	328	GLN	2.4
1	A	235	GLY	2.4
1	A	164	LEU	2.4
1	A	71	TYR	2.4
1	A	98	GLY	2.4
1	A	204	VAL	2.4
1	A	294	ASN	2.4
1	A	170	LEU	2.4
1	A	74	SER	2.4
1	A	334	ALA	2.3
1	A	234	PRO	2.3
1	A	166	THR	2.3
1	A	111	LEU	2.3
1	A	173	LEU	2.3
1	A	311	LEU	2.3
1	A	268	GLY	2.3
1	A	243	ALA	2.3
1	A	151	VAL	2.3
1	A	320	SER	2.3
1	A	332	TRP	2.3
1	A	91	LEU	2.3
1	A	149	TYR	2.3
1	A	342	THR	2.3
1	A	117	GLY	2.3
1	A	150	TYR	2.2
1	A	237	TYR	2.2
1	A	287	ALA	2.2
1	A	136	THR	2.2
1	A	305	HIS	2.2
1	A	115	THR	2.2
1	A	128	ALA	2.1
1	A	240	SER	2.1
1	A	142	MET	2.1
1	A	285	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	160	PRO	2.1
1	A	66	LEU	2.1
1	A	232	LEU	2.1
1	A	253	GLN	2.1
1	A	292	GLN	2.1
1	A	343	ALA	2.1
1	A	245	THR	2.1
1	A	242	GLU	2.1
1	A	252	SER	2.1
1	A	93	PRO	2.1
1	A	122	ALA	2.1
1	A	231	THR	2.0
1	A	103	ASP	2.0
1	A	165	GLY	2.0
1	A	167	GLY	2.0
1	A	163	THR	2.0
1	A	324	LEU	2.0
1	A	273	SER	2.0
1	A	106	ASN	2.0
1	A	218	ASP	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	HG	A	403	1/1	0.95	0.09	40,40,40,40	0
2	HG	A	402	1/1	0.96	0.07	47,47,47,47	1
2	HG	A	401	1/1	0.96	0.07	43,43,43,43	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HG	A	404	1/1	0.98	0.09	41,41,41,41	1

6.5 Other polymers [i](#)

There are no such residues in this entry.