



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:02 AM UTC

PDB ID : 1XZ6 / pdb_00001xz6
Title : Mutant ABO(H) blood group glycosyltransferase 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 : 2004-11-11
Resolution : 1.55 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

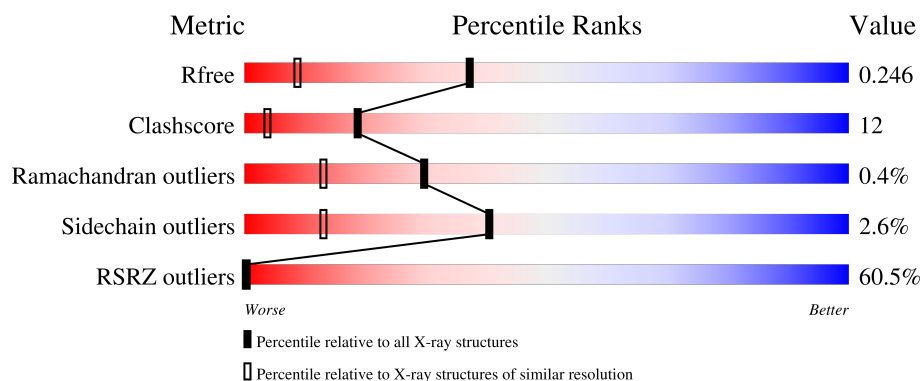
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	54% 72% 16% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2404 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
			2153	1400	369	374	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	268	ARG	GLY	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		

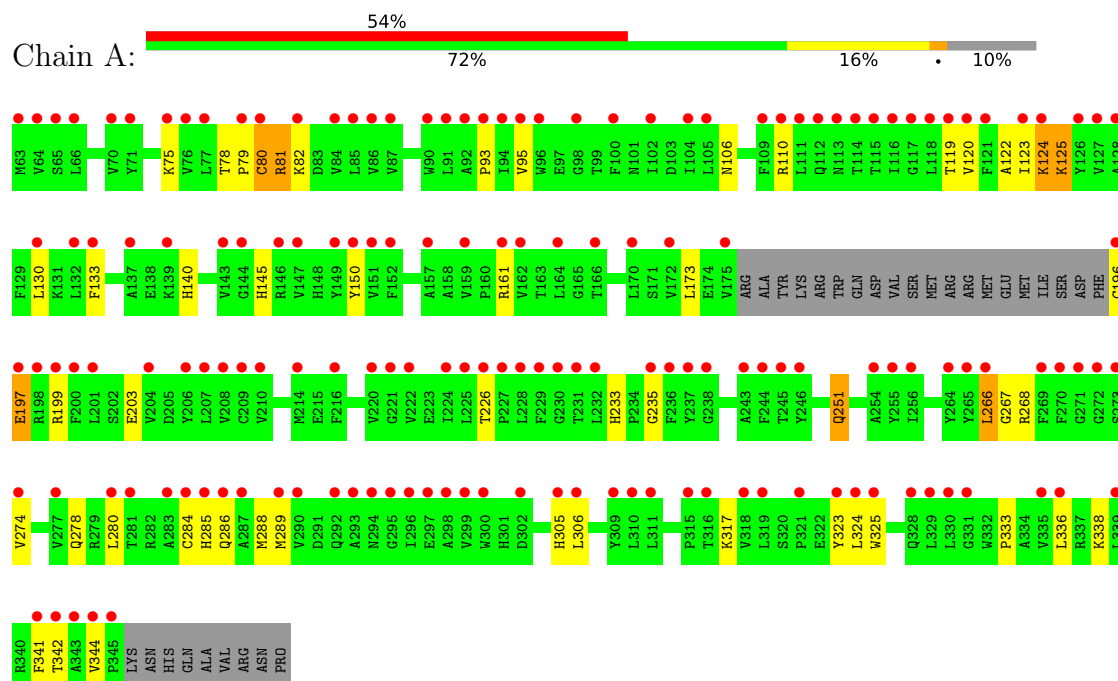
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	247	Total	O	0	0
			247	247		

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	52.90Å 150.90Å 79.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.55 20.00 – 1.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.55) 90.4 (20.00-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.243 0.224 , 0.246	Depositor DCC
R_{free} test set	291 reflections (0.66%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2404	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 5.06% 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: 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	0.35	0/2214	0.91	6/3010 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	VAL	N-CA-C	6.74	118.16	107.98
1	A	267	GLY	N-CA-C	-6.44	106.67	114.66
1	A	268	ARG	N-CA-C	6.38	120.00	112.72
1	A	124	LYS	CB-CA-C	-5.46	110.26	116.54
1	A	130	LEU	N-CA-C	5.21	116.95	111.28
1	A	342	THR	N-CA-C	5.10	116.94	109.24

There are no chirality outliers.

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	2153	0	2142	51	0
2	A	4	0	0	0	0
3	A	247	0	0	4	0
All	All	2404	0	2142	51	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 12.

All (51) 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	1.26	0.98
1:A:233:HIS:HD2	1:A:235:GLY:H	1.15	0.92
1:A:123:ILE:HG22	1:A:124:LYS:HG3	1.62	0.81
1:A:226:THR:HG21	1:A:317:LYS:HB2	1.69	0.74
1:A:251:GLN:NE2	1:A:251:GLN:H	1.89	0.70
1:A:284:CYS:HB2	3:A:691:HOH:O	1.96	0.65
1:A:285:HIS:O	1:A:289:MET:HG3	1.98	0.63
1:A:233:HIS:HA	1:A:266:LEU:HD22	1.81	0.61
1:A:266:LEU:HG	1:A:324:LEU:HD13	1.81	0.60
1:A:233:HIS:CD2	1:A:235:GLY:H	2.07	0.59
1:A:75:LYS:HB2	1:A:78:THR:HB	1.84	0.58
1:A:233:HIS:HA	1:A:266:LEU:CD2	2.33	0.58
1:A:274:VAL:O	1:A:278:GLN:HG3	2.06	0.55
1:A:325:TRP:CZ3	1:A:336:LEU:HD11	2.44	0.53
1:A:122:ALA:C	1:A:123:ILE:HD12	2.35	0.52
1:A:286:GLN:HA	1:A:289:MET:CE	2.40	0.52
1:A:93:PRO:HG2	1:A:317:LYS:HG2	1.92	0.51
1:A:75:LYS:CB	1:A:78:THR:HB	2.41	0.51
1:A:120:VAL:HG11	1:A:133:PHE:CZ	2.47	0.50
1:A:123:ILE:HD12	1:A:123:ILE:N	2.27	0.50
1:A:123:ILE:CG2	1:A:124:LYS:HG3	2.38	0.48
1:A:80:CYS:O	1:A:81:ARG:HB2	2.13	0.48
1:A:199:ARG:O	1:A:203:GLU:HG3	2.13	0.48
1:A:80:CYS:O	1:A:81:ARG:CB	2.62	0.47
1:A:286:GLN:HA	1:A:289:MET:HE3	1.96	0.47
1:A:106:ASN:OD1	1:A:145:HIS:HE1	1.97	0.47
1:A:173:LEU:HD22	1:A:173:LEU:N	2.29	0.47
1:A:140:HIS:HD2	3:A:722:HOH:O	1.97	0.46
1:A:124:LYS:HB3	1:A:125:LYS:HD3	1.97	0.46
1:A:125:LYS:H	1:A:125:LYS:CD	2.08	0.46
1:A:251:GLN:H	1:A:251:GLN:HE21	1.61	0.46
1:A:196:CYS:SG	1:A:199:ARG:HB2	2.57	0.45
1:A:79:PRO:HD2	1:A:82:LYS:HE2	1.98	0.44
1:A:196:CYS:C	1:A:197:GLU:OE1	2.61	0.44
1:A:280:LEU:C	1:A:280:LEU:HD23	2.43	0.44
1:A:226:THR:HB	1:A:317:LYS:HD2	1.99	0.44
1:A:288:MET:HG2	1:A:305:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:VAL:HG23	1:A:344:VAL:O	2.16	0.44
1:A:323:TYR:O	1:A:341:PHE:HB3	2.19	0.43
1:A:325:TRP:CH2	1:A:336:LEU:HD11	2.54	0.43
1:A:124:LYS:CB	1:A:125:LYS:HD3	2.49	0.42
1:A:305:HIS:HE1	3:A:530:HOH:O	2.01	0.42
1:A:110:ARG:HD2	1:A:110:ARG:HA	1.90	0.42
1:A:333:PRO:HD2	1:A:336:LEU:HD12	2.02	0.41
1:A:306:LEU:C	1:A:306:LEU:HD23	2.45	0.41
1:A:251:GLN:NE2	1:A:251:GLN:N	2.63	0.41
1:A:338:LYS:HE3	3:A:723:HOH:O	2.21	0.41
1:A:233:HIS:CA	1:A:266:LEU:HD22	2.50	0.41
1:A:284:CYS:O	1:A:288:MET:HG3	2.21	0.41
1:A:324:LEU:HD23	1:A:324:LEU:C	2.46	0.40
1:A:119:THR:HG22	1:A:150:TYR:HB2	2.04	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	259/292 (89%)	253 (98%)	5 (2%)	1 (0%)	30 13

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ARG

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	234/261 (90%)	228 (97%)	6 (3%)	40 13

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	251	GLN
1	A	266	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	113	ASN
1	A	140	HIS
1	A	145	HIS
1	A	169	GLN
1	A	233	HIS
1	A	251	GLN
1	A	253	GLN
1	A	275	GLN
1	A	285	HIS
1	A	305	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%)	2.22	159 (60%) 0 0	14, 24, 40, 59	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	CYS	7.6
1	A	196	CYS	5.4
1	A	64	VAL	5.3
1	A	63	MET	5.2
1	A	345	PRO	4.2
1	A	161	ARG	4.0
1	A	266	LEU	3.9
1	A	209	CYS	3.9
1	A	293	ALA	3.9
1	A	299	VAL	3.7
1	A	175	VAL	3.7
1	A	281	THR	3.6
1	A	336	LEU	3.6
1	A	286	GLN	3.6
1	A	95	VAL	3.5
1	A	113	ASN	3.5
1	A	121	PHE	3.4
1	A	123	ILE	3.4
1	A	292	GLN	3.4
1	A	255	TYR	3.4
1	A	170	LEU	3.4
1	A	339	LEU	3.4
1	A	224	ILE	3.3
1	A	222	VAL	3.3
1	A	147	VAL	3.3
1	A	92	ALA	3.3
1	A	329	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	342	THR	3.2
1	A	120	VAL	3.2
1	A	270	PHE	3.1
1	A	87	VAL	3.1
1	A	335	VAL	3.1
1	A	137	ALA	3.1
1	A	236	PHE	3.0
1	A	172	VAL	3.0
1	A	127	VAL	2.9
1	A	274	VAL	2.9
1	A	166	THR	2.9
1	A	90	TRP	2.9
1	A	96	TRP	2.9
1	A	128	ALA	2.9
1	A	117	GLY	2.9
1	A	79	PRO	2.9
1	A	319	LEU	2.9
1	A	112	GLN	2.9
1	A	289	MET	2.9
1	A	199	ARG	2.9
1	A	102	ILE	2.8
1	A	309	TYR	2.8
1	A	116	ILE	2.8
1	A	126	TYR	2.8
1	A	228	LEU	2.8
1	A	197	GLU	2.8
1	A	283	ALA	2.8
1	A	152	PHE	2.8
1	A	94	ILE	2.8
1	A	328	GLN	2.8
1	A	86	VAL	2.7
1	A	265	TYR	2.7
1	A	91	LEU	2.7
1	A	235	GLY	2.7
1	A	198	ARG	2.7
1	A	306	LEU	2.7
1	A	159	VAL	2.7
1	A	277	VAL	2.7
1	A	300	TRP	2.7
1	A	256	ILE	2.7
1	A	98	GLY	2.6
1	A	84	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	290	VAL	2.6
1	A	302	ASP	2.6
1	A	318	VAL	2.6
1	A	325	TRP	2.6
1	A	284	CYS	2.6
1	A	298	ALA	2.6
1	A	130	LEU	2.6
1	A	341	PHE	2.6
1	A	210	VAL	2.6
1	A	220	VAL	2.6
1	A	321	PRO	2.6
1	A	75	LYS	2.5
1	A	139	LYS	2.5
1	A	206	TYR	2.5
1	A	229	PHE	2.5
1	A	330	LEU	2.5
1	A	146	ARG	2.5
1	A	143	VAL	2.5
1	A	344	VAL	2.5
1	A	132	LEU	2.5
1	A	225	LEU	2.5
1	A	200	PHE	2.5
1	A	114	THR	2.5
1	A	118	LEU	2.5
1	A	201	LEU	2.5
1	A	285	HIS	2.5
1	A	254	ALA	2.4
1	A	104	ILE	2.4
1	A	296	ILE	2.4
1	A	310	LEU	2.4
1	A	109	PHE	2.4
1	A	294	ASN	2.4
1	A	226	THR	2.4
1	A	316	THR	2.4
1	A	100	PHE	2.4
1	A	244	PHE	2.4
1	A	243	ALA	2.4
1	A	77	LEU	2.4
1	A	105	LEU	2.4
1	A	111	LEU	2.4
1	A	324	LEU	2.4
1	A	269	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	207	LEU	2.3
1	A	208	VAL	2.3
1	A	295	GLY	2.3
1	A	323	TYR	2.3
1	A	162	VAL	2.3
1	A	119	THR	2.3
1	A	110	ARG	2.3
1	A	230	GLY	2.3
1	A	271	GLY	2.3
1	A	124	LYS	2.3
1	A	85	LEU	2.3
1	A	297	GLU	2.3
1	A	133	PHE	2.2
1	A	231	THR	2.2
1	A	232	LEU	2.2
1	A	311	LEU	2.2
1	A	204	VAL	2.2
1	A	66	LEU	2.2
1	A	264	TYR	2.2
1	A	343	ALA	2.2
1	A	315	PRO	2.2
1	A	245	THR	2.2
1	A	216	PHE	2.2
1	A	151	VAL	2.2
1	A	157	ALA	2.1
1	A	238	GLY	2.1
1	A	246	TYR	2.1
1	A	70	VAL	2.1
1	A	93	PRO	2.1
1	A	227	PRO	2.1
1	A	331	GLY	2.1
1	A	149	TYR	2.1
1	A	305	HIS	2.1
1	A	287	ALA	2.1
1	A	280	LEU	2.1
1	A	144	GLY	2.1
1	A	221	GLY	2.1
1	A	272	GLY	2.1
1	A	115	THR	2.0
1	A	76	VAL	2.0
1	A	164	LEU	2.0
1	A	71	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	150	TYR	2.0
1	A	82	LYS	2.0
1	A	214	MET	2.0
1	A	65	SER	2.0
1	A	273	SER	2.0
1	A	237	TYR	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($\text{\AA}^2$)	Q<0.9
2	HG	A	403	1/1	0.91	0.12	46,46,46,46	0
2	HG	A	402	1/1	0.94	0.09	57,57,57,57	1
2	HG	A	401	1/1	0.94	0.07	44,44,44,44	1
2	HG	A	404	1/1	0.94	0.27	66,66,66,66	1

6.5 Other polymers [i](#)

There are no such residues in this entry.