



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7LAW / pdb_00007law
Title : crystal structure of GTR complex with GTR-L
Authors : Longenecker, K.L.; Rogers, B.; Bigelow, L.; Judge, R.A.; Alvarez, H.
Deposited on : 2021-01-07
Resolution : 2.75 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

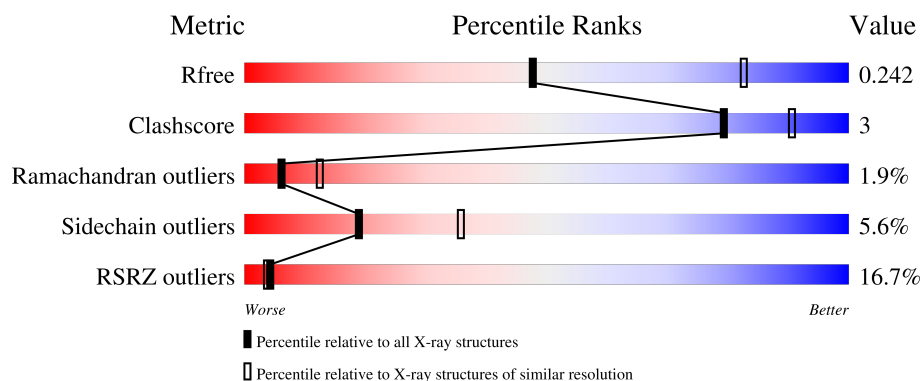
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	128	5% 88% 6% • 5%
1	B	128	9% 84% 11% 5%
2	R	147	18% 52% 12% • 35%
2	S	147	18% 52% 14% 35%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3388 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 Tumor necrosis factor ligand superfamily member 18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			974	628	160	181	5			
1	B	122	Total	C	N	O	S	0	0	0
			974	628	160	181	5			

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	96	Total	C	N	O	S	0	0	0
			668	409	123	125	11			
2	S	96	Total	C	N	O	S	0	0	0
			668	409	123	125	11			

There are 22 discrepancies between the modelled and reference sequences:

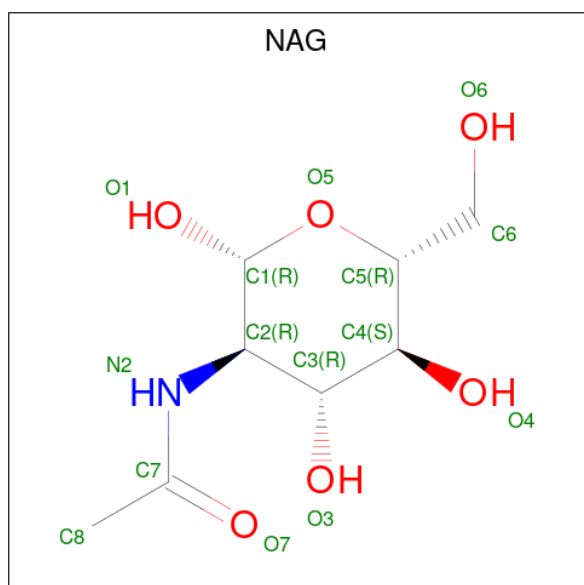
Chain	Residue	Modelled	Actual	Comment	Reference
R	162	ALA	-	expression tag	UNP Q9Y5U5
R	163	ALA	-	expression tag	UNP Q9Y5U5
R	164	ALA	-	expression tag	UNP Q9Y5U5
R	165	HIS	-	expression tag	UNP Q9Y5U5
R	166	HIS	-	expression tag	UNP Q9Y5U5
R	167	HIS	-	expression tag	UNP Q9Y5U5
R	168	HIS	-	expression tag	UNP Q9Y5U5
R	169	HIS	-	expression tag	UNP Q9Y5U5
R	170	HIS	-	expression tag	UNP Q9Y5U5
R	171	HIS	-	expression tag	UNP Q9Y5U5
R	172	HIS	-	expression tag	UNP Q9Y5U5
S	162	ALA	-	expression tag	UNP Q9Y5U5
S	163	ALA	-	expression tag	UNP Q9Y5U5
S	164	ALA	-	expression tag	UNP Q9Y5U5
S	165	HIS	-	expression tag	UNP Q9Y5U5
S	166	HIS	-	expression tag	UNP Q9Y5U5

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Chain	Residue	Modelled	Actual	Comment	Reference
S	167	HIS	-	expression tag	UNP Q9Y5U5
S	168	HIS	-	expression tag	UNP Q9Y5U5
S	169	HIS	-	expression tag	UNP Q9Y5U5
S	170	HIS	-	expression tag	UNP Q9Y5U5
S	171	HIS	-	expression tag	UNP Q9Y5U5
S	172	HIS	-	expression tag	UNP Q9Y5U5

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	R	1	Total	C	N	O	0	0
			14	8	1	5		
3	S	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	18	Total	O	0	0
			18	18		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	3	Total	O	0	0
			3	3		
4	S	8	Total	O	0	0
			8	8		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	172.66Å 172.66Å 172.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.09 – 2.75 122.09 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.5 (122.09-2.75) 96.5 (122.09-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.7 (18-SEP-2020)	Depositor
R, R_{free}	0.229 , 0.236 0.233 , 0.242	Depositor DCC
R_{free} test set	1099 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	79.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.025 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3388	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: NAG

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	0.73	0/999	0.97	0/1360
1	B	0.75	1/999 (0.1%)	0.99	0/1360
2	R	0.74	0/691	1.18	5/933 (0.5%)
2	S	0.76	0/691	1.16	5/933 (0.5%)
All	All	0.74	1/3380 (0.0%)	1.06	10/4586 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	LYS	CA-C	5.26	1.56	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	108	PHE	CA-C-N	7.22	127.16	122.18
2	S	108	PHE	C-N-CA	7.22	127.16	122.18
2	R	108	PHE	CA-C-N	7.07	127.06	122.18
2	R	108	PHE	C-N-CA	7.07	127.06	122.18
2	S	137	PHE	N-CA-C	-6.61	100.67	110.46
2	R	73	MET	CA-C-N	6.27	133.51	121.54
2	R	73	MET	C-N-CA	6.27	133.51	121.54
2	R	146	ASN	CA-CB-CG	5.79	118.39	112.60
2	S	146	ASN	CA-CB-CG	5.62	118.22	112.60
2	S	142	VAL	N-CA-C	-5.39	106.44	111.45

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	974	0	961	4	0
1	B	974	0	961	7	0
2	R	668	0	555	5	0
2	S	668	0	555	5	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	R	14	0	13	0	0
3	S	14	0	13	0	0
4	A	19	0	0	1	0
4	B	18	0	0	0	0
4	R	3	0	0	0	0
4	S	8	0	0	0	0
All	All	3388	0	3084	17	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 3.

All (17) 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:71:MET:HE1	1:A:79:VAL:HG23	1.86	0.56
1:B:143:HIS:CE1	1:B:176:ILE:HG23	2.40	0.56
2:R:139:PHE:CZ	2:S:132:THR:HG21	2.42	0.55
1:B:71:MET:HE1	1:B:79:VAL:HG23	1.90	0.53
1:B:143:HIS:HE1	1:B:176:ILE:HG23	1.76	0.51
1:A:81:LYS:HD2	1:B:177:SER:HA	1.93	0.50
1:A:82:VAL:HG22	1:B:144:VAL:HG11	1.92	0.50
2:R:97:GLY:HA2	2:R:147:LYS:O	2.13	0.49
2:R:94:CYS:O	2:R:124:HIS:HA	2.13	0.49
2:S:94:CYS:O	2:S:124:HIS:HA	2.14	0.48
1:B:143:HIS:CE1	1:B:176:ILE:CG2	2.99	0.45
2:S:119:THR:HA	2:S:130:PRO:HA	2.00	0.44
2:R:155:PRO:HD2	2:S:155:PRO:HG3	1.99	0.44
2:R:78:GLU:HG2	2:R:93:PRO:HB3	2.00	0.42
1:A:174:GLN:HG2	4:A:309:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:143:PHE:CD1	2:S:144:PRO:HD2	2.55	0.41
1:B:141:GLU:HG3	1:B:176:ILE:HD13	2.03	0.41

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	120/128 (94%)	115 (96%)	5 (4%)	0	100	100
1	B	120/128 (94%)	116 (97%)	3 (2%)	1 (1%)	16	30
2	R	94/147 (64%)	82 (87%)	7 (7%)	5 (5%)	1	2
2	S	94/147 (64%)	81 (86%)	11 (12%)	2 (2%)	5	11
All	All	428/550 (78%)	394 (92%)	26 (6%)	8 (2%)	6	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	64	GLU
2	R	74	CYS
2	S	64	GLU
1	B	73	SER
2	R	70	TRP
2	S	70	TRP
2	R	73	MET
2	R	86	CYS

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	109/114 (96%)	104 (95%)	5 (5%)	24	45
1	B	109/114 (96%)	104 (95%)	5 (5%)	24	45
2	R	69/120 (58%)	65 (94%)	4 (6%)	18	34
2	S	69/120 (58%)	63 (91%)	6 (9%)	9	18
All	All	356/468 (76%)	336 (94%)	20 (6%)	19	36

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	81	LYS
1	A	106	ASN
1	A	135	ASN
1	A	158	VAL
1	B	81	LYS
1	B	106	ASN
1	B	135	ASN
1	B	158	VAL
1	B	174	GLN
2	R	75	VAL
2	R	111	GLN
2	R	113	ILE
2	R	154	VAL
2	S	75	VAL
2	S	105	LYS
2	S	111	GLN
2	S	113	ILE
2	S	141	THR
2	S	154	VAL

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	134	GLN
1	A	143	HIS
1	A	162	ASN

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Mol	Chain	Res	Type
1	B	134	GLN
1	B	143	HIS
1	B	162	ASN
2	R	76	GLN
2	R	92	HIS
2	S	80	HIS
2	S	91	HIS
2	S	92	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

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	$\# Z > 2$
3	NAG	A	201	1	14,14,15	0.34	0	17,19,21	0.67	1 (5%)
3	NAG	B	201	1	14,14,15	0.38	0	17,19,21	0.66	0
3	NAG	R	501	2	14,14,15	0.37	0	17,19,21	0.72	1 (5%)
3	NAG	S	501	2	14,14,15	0.38	0	17,19,21	0.89	2 (11%)

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
3	NAG	A	201	1	-	0/6/23/26	0/1/1/1
3	NAG	B	201	1	-	0/6/23/26	0/1/1/1
3	NAG	R	501	2	-	0/6/23/26	0/1/1/1
3	NAG	S	501	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	NAG	C1-O5-C5	2.36	115.35	112.19
3	R	501	NAG	C1-O5-C5	2.24	115.19	112.19
3	S	501	NAG	C1-O5-C5	2.23	115.18	112.19
3	S	501	NAG	O5-C1-C2	-2.09	108.06	111.29

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	122/128 (95%)	0.42	7 (5%)	29 29	56, 71, 96, 109	0
1	B	122/128 (95%)	0.56	12 (9%)	13 12	51, 73, 94, 116	0
2	R	96/147 (65%)	1.56	27 (28%)	1 1	70, 89, 132, 133	0
2	S	96/147 (65%)	1.43	27 (28%)	1 1	72, 90, 110, 115	0
All	All	436/550 (79%)	0.93	73 (16%)	4 4	51, 80, 111, 133	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	66	CYS	7.6
2	S	66	CYS	6.8
2	S	68	SER	6.2
1	B	177	SER	6.1
2	R	61	TYR	6.1
2	S	67	CYS	6.1
2	R	67	CYS	5.6
2	R	72	CYS	5.4
2	R	68	SER	5.2
2	R	71	ASP	5.1
2	R	73	MET	5.0
2	S	70	TRP	4.8
2	R	101	GLN	4.7
2	S	72	CYS	4.5
2	R	63	GLY	4.1
2	R	70	TRP	4.1
2	S	71	ASP	4.0
2	S	101	GLN	4.0
1	B	176	ILE	3.9
2	R	75	VAL	3.8
2	S	61	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	176	ILE	3.7
1	B	174	GLN	3.6
2	R	103	GLN	3.6
1	B	73	SER	3.4
1	A	177	SER	3.3
2	S	63	GLY	3.2
2	S	69	GLU	3.2
2	R	77	PRO	3.2
2	R	156	GLY	3.2
2	S	113	ILE	3.1
2	S	111	GLN	3.1
2	R	62	PRO	3.0
1	B	175	PHE	3.0
2	S	77	PRO	2.9
1	A	110	VAL	2.8
2	R	110	PHE	2.8
2	R	92	HIS	2.7
1	B	172	ASN	2.7
1	B	132	LYS	2.7
1	A	109	ASP	2.7
2	R	93	PRO	2.7
2	R	69	GLU	2.6
1	A	175	PHE	2.6
2	S	126	GLY	2.5
2	S	127	HIS	2.5
2	R	102	SER	2.5
2	S	128	CYS	2.4
2	S	73	MET	2.4
2	S	123	GLY	2.4
1	A	172	ASN	2.4
1	B	173	PRO	2.4
2	S	75	VAL	2.4
2	R	74	CYS	2.4
2	R	135	THR	2.3
2	S	110	PHE	2.3
2	R	127	HIS	2.3
2	S	129	LYS	2.3
2	R	136	GLN	2.3
1	B	103	PRO	2.2
1	A	174	GLN	2.2
2	S	102	SER	2.2
2	S	114	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	145	GLY	2.1
1	B	110	VAL	2.1
2	R	125	GLU	2.1
2	R	141	THR	2.1
2	R	79	PHE	2.1
2	S	147	LYS	2.0
1	B	71	MET	2.0
2	S	62	PRO	2.0
2	S	135	THR	2.0
2	S	142	VAL	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
3	NAG	B	201	14/15	0.60	0.17	109,111,111,111	0
3	NAG	S	501	14/15	0.69	0.16	93,94,95,95	0
3	NAG	R	501	14/15	0.70	0.18	97,99,99,100	0
3	NAG	A	201	14/15	0.77	0.14	106,109,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.