



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1D4N  
Title : HUMAN SERUM TRANSFERRIN  
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Deposited on : 1999-10-04  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

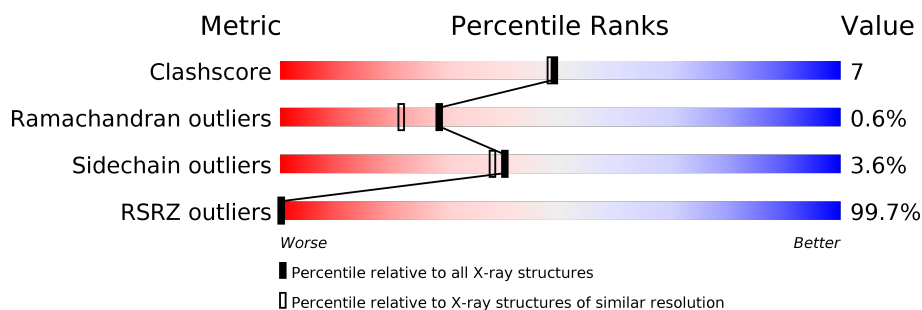
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	329	<div> <div>100%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>

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	CO3	A	338	-	-	-	X
3	FE	A	339	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2690 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.

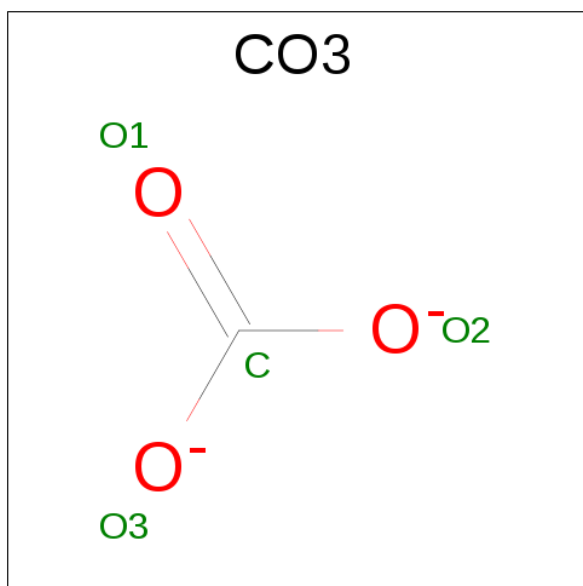
- Molecule 1 is a protein called TRANSFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	329	2550	1611	435	483	21	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	GLU	HIS	ENGINEERED	UNP P02787

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	1	3	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Fe 1	0	0

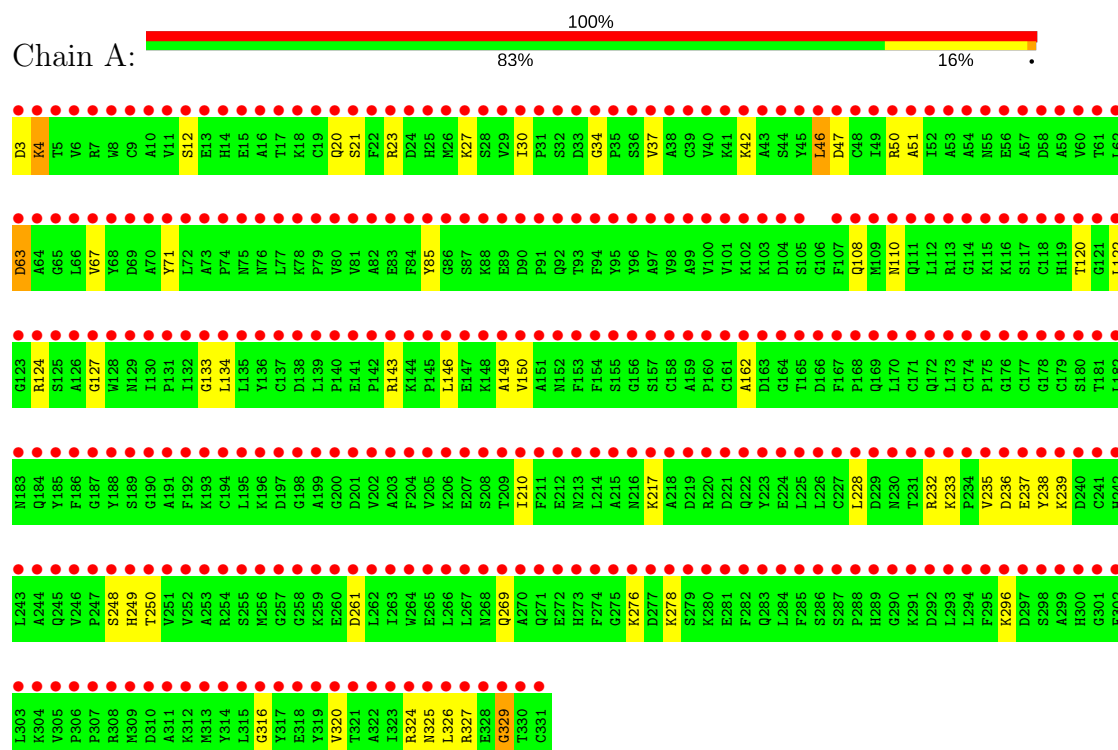
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total 135	O 135	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: TRANSFERRIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.03Å 57.91Å 135.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.00 – 2.00 31.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (32.00-2.00) 87.6 (31.94-2.00)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.59 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.179 , 0.218 0.185 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	21.5	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2690	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CO3, FE

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	0.46	0/2610	0.63	0/3527

There are no bond length outliers.

There are no bond angle outliers.

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	2550	0	2466	34	0
2	A	4	0	0	1	0
3	A	1	0	0	0	0
4	A	135	0	0	0	0
All	All	2690	0	2466	34	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 7.

All (34) 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:3:ASP:O	1:A:4:LYS:HB2	1.82	0.80
1:A:67:VAL:HG21	1:A:250:THR:CG2	2.29	0.62
1:A:85:TYR:HE2	1:A:248:SER:HB3	1.64	0.62
1:A:325:ASN:O	1:A:329:GLY:HA3	2.05	0.56
1:A:63:ASP:HA	1:A:249:HIS:CD2	2.41	0.55
1:A:124:ARG:NH2	2:A:338:CO3:O2	2.40	0.55
1:A:46:LEU:O	1:A:50:ARG:HG2	2.06	0.55
1:A:134:LEU:HD13	1:A:228:LEU:HD21	1.90	0.54
1:A:23:ARG:HG3	1:A:37:VAL:O	2.11	0.51
1:A:85:TYR:CE2	1:A:248:SER:HB3	2.45	0.51
1:A:122:LEU:HD22	1:A:162:ALA:HA	1.92	0.50
1:A:23:ARG:HG2	1:A:27:LYS:HE3	1.94	0.50
1:A:249:HIS:CE1	1:A:296:LYS:HD2	2.48	0.48
1:A:210:ILE:HD13	1:A:235:VAL:HG11	1.96	0.48
1:A:316:GLY:O	1:A:320:VAL:HG23	2.14	0.47
1:A:320:VAL:O	1:A:324:ARG:HG3	2.14	0.47
1:A:133:GLY:HA2	1:A:326:LEU:HD13	1.97	0.46
1:A:67:VAL:HG21	1:A:250:THR:HG23	1.99	0.45
1:A:143:ARG:HA	1:A:149:ALA:HB2	1.98	0.45
1:A:108:GLN:HB2	1:A:110:ASN:OD1	2.18	0.44
1:A:108:GLN:HA	1:A:108:GLN:NE2	2.32	0.44
1:A:233:LYS:HD3	1:A:237:GLU:OE1	2.17	0.44
1:A:42:LYS:HD2	1:A:47:ASP:HB3	2.00	0.44
1:A:146:LEU:O	1:A:150:VAL:HG23	2.19	0.43
1:A:238:TYR:CE1	1:A:239:LYS:HG3	2.55	0.42
1:A:42:LYS:HE3	1:A:51:ALA:HB2	2.01	0.42
1:A:30:ILE:CD1	1:A:269:GLN:NE2	2.83	0.42
1:A:30:ILE:CG2	1:A:34:GLY:HA3	2.50	0.41
1:A:108:GLN:HE22	1:A:232:ARG:HG3	1.86	0.41
1:A:120:THR:OG1	1:A:127:GLY:HA3	2.21	0.41
1:A:42:LYS:HB3	1:A:47:ASP:HB2	2.02	0.41
1:A:261:ASP:OD1	1:A:261:ASP:N	2.54	0.41
1:A:278:LYS:HE2	1:A:278:LYS:HB3	1.74	0.41
1:A:85:TYR:HE2	1:A:248:SER:CB	2.33	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	327/329 (99%)	307 (94%)	18 (6%)	2 (1%)	28	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	329	GLY

### 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	274/274 (100%)	264 (96%)	10 (4%)	40	38

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	20	GLN
1	A	21	SER
1	A	46	LEU
1	A	63	ASP
1	A	71	TYR
1	A	217	LYS
1	A	236	ASP
1	A	276	LYS

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Mol	Chain	Res	Type
1	A	327	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	108	GLN
1	A	152	ASN
1	A	269	GLN
1	A	325	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	CO3	A	338	3	0,3,3	0.00	-	0,3,3	0.00	-

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	CO3	A	338	3	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	338	CO3	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	329/329 (100%)	11.91	328 (99%) 0 0	11, 22, 54, 83	0

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	ASN	44.8
1	A	284	LEU	42.2
1	A	209	THR	37.8
1	A	282	PHE	37.6
1	A	192	PHE	37.3
1	A	330	THR	35.8
1	A	229	ASP	35.7
1	A	200	GLY	34.3
1	A	182	LEU	32.6
1	A	303	LEU	31.4
1	A	228	LEU	31.1
1	A	205	VAL	31.0
1	A	135	LEU	30.1
1	A	171	CYS	29.4
1	A	73	ALA	27.3
1	A	210	ILE	26.9
1	A	283	GLN	26.7
1	A	75	ASN	26.6
1	A	43	ALA	26.6
1	A	178	GLY	26.4
1	A	137	CYS	26.3
1	A	288	PRO	26.1
1	A	309	MET	25.5
1	A	117	SER	25.5
1	A	213	ASN	25.3
1	A	40	VAL	24.6
1	A	194	CYS	24.6

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Mol	Chain	Res	Type	RSRZ
1	A	199	ALA	24.4
1	A	91	PRO	23.9
1	A	166	ASP	23.3
1	A	263	ILE	23.0
1	A	90	ASP	23.0
1	A	128	TRP	22.4
1	A	98	VAL	22.1
1	A	211	PHE	21.8
1	A	89	GLU	21.8
1	A	308	ARG	21.6
1	A	227	CYS	21.5
1	A	87	SER	21.4
1	A	304	LYS	21.1
1	A	237	GLU	20.7
1	A	84	PHE	20.6
1	A	203	ALA	20.3
1	A	233	LYS	20.2
1	A	275	GLY	19.8
1	A	305	VAL	19.5
1	A	35	PRO	19.2
1	A	195	LEU	19.2
1	A	52	ILE	19.0
1	A	138	ASP	18.7
1	A	136	TYR	18.5
1	A	163	ASP	18.5
1	A	236	ASP	18.4
1	A	202	VAL	18.4
1	A	22	PHE	18.2
1	A	300	HIS	17.9
1	A	5	THR	17.9
1	A	34	GLY	17.9
1	A	242	HIS	17.9
1	A	31	PRO	17.8
1	A	134	LEU	17.7
1	A	131	PRO	17.7
1	A	165	THR	17.6
1	A	239	LYS	17.5
1	A	240	ASP	17.5
1	A	310	ASP	17.4
1	A	81	VAL	17.3
1	A	38	ALA	17.1
1	A	201	ASP	17.1

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Mol	Chain	Res	Type	RSRZ
1	A	234	PRO	16.9
1	A	16	ALA	16.9
1	A	259	LYS	16.9
1	A	177	CYS	16.9
1	A	329	GLY	16.8
1	A	42	LYS	16.7
1	A	7	ARG	16.3
1	A	274	PHE	16.1
1	A	231	THR	16.1
1	A	173	LEU	15.9
1	A	68	TYR	15.9
1	A	3	ASP	15.6
1	A	243	LEU	15.6
1	A	331	CYS	15.5
1	A	196	LYS	15.5
1	A	6	VAL	15.5
1	A	197	ASP	15.4
1	A	72	LEU	15.3
1	A	51	ALA	15.2
1	A	71	TYR	15.0
1	A	46	LEU	14.7
1	A	198	GLY	14.7
1	A	255	SER	14.6
1	A	76	ASN	14.5
1	A	37	VAL	14.5
1	A	61	THR	14.4
1	A	193	LYS	14.4
1	A	206	LYS	14.3
1	A	172	GLN	14.2
1	A	328	GLU	14.2
1	A	113	ARG	14.1
1	A	287	SER	14.0
1	A	156	GLY	13.9
1	A	32	SER	13.9
1	A	169	GLN	13.9
1	A	183	ASN	13.8
1	A	168	PRO	13.7
1	A	324	ARG	13.5
1	A	295	PHE	13.5
1	A	170	LEU	13.4
1	A	56	GLU	13.4
1	A	244	ALA	13.3

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Mol	Chain	Res	Type	RSRZ
1	A	141	GLU	13.3
1	A	175	PRO	13.2
1	A	176	GLY	13.2
1	A	47	ASP	13.0
1	A	289	HIS	13.0
1	A	157	SER	12.8
1	A	312	LYS	12.8
1	A	39	CYS	12.6
1	A	25	HIS	12.4
1	A	238	TYR	12.4
1	A	179	CYS	12.3
1	A	55	ASN	12.3
1	A	77	LEU	12.2
1	A	285	PHE	12.1
1	A	276	LYS	12.1
1	A	96	TYR	12.1
1	A	24	ASP	12.0
1	A	127	GLY	12.0
1	A	294	LEU	11.9
1	A	280	LYS	11.8
1	A	181	THR	11.7
1	A	8	TRP	11.7
1	A	74	PRO	11.6
1	A	261	ASP	11.6
1	A	88	LYS	11.6
1	A	326	LEU	11.6
1	A	317	TYR	11.4
1	A	41	LYS	11.3
1	A	129	ASN	11.3
1	A	154	PHE	11.3
1	A	82	ALA	10.9
1	A	313	MET	10.8
1	A	185	TYR	10.7
1	A	277	ASP	10.7
1	A	167	PHE	10.6
1	A	264	TRP	10.5
1	A	125	SER	10.5
1	A	204	PHE	10.5
1	A	118	CYS	10.5
1	A	30	ILE	10.4
1	A	33	ASP	10.4
1	A	112	LEU	10.4

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Mol	Chain	Res	Type	RSRZ
1	A	257	GLY	10.4
1	A	191	ALA	10.4
1	A	100	VAL	10.3
1	A	164	GLY	10.3
1	A	12	SER	10.2
1	A	94	PHE	10.2
1	A	222	GLN	10.2
1	A	28	SER	10.0
1	A	132	ILE	10.0
1	A	235	VAL	10.0
1	A	17	THR	9.9
1	A	241	CYS	9.9
1	A	258	GLY	9.8
1	A	50	ARG	9.8
1	A	116	LYS	9.8
1	A	225	LEU	9.6
1	A	14	HIS	9.5
1	A	215	ALA	9.5
1	A	208	SER	9.5
1	A	103	LYS	9.4
1	A	80	VAL	9.3
1	A	19	CYS	9.3
1	A	67	VAL	9.3
1	A	85	TYR	9.2
1	A	189	SER	9.1
1	A	48	CYS	9.1
1	A	219	ASP	9.1
1	A	271	GLN	9.0
1	A	325	ASN	8.8
1	A	147	GLU	8.7
1	A	101	VAL	8.7
1	A	323	ILE	8.5
1	A	63	ASP	8.4
1	A	62	LEU	8.4
1	A	299	ALA	8.4
1	A	226	LEU	8.4
1	A	92	GLN	8.4
1	A	13	GLU	8.3
1	A	93	THR	8.3
1	A	281	GLU	8.2
1	A	9	CYS	8.2
1	A	249	HIS	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	159	ALA	8.1
1	A	256	MET	8.1
1	A	190	GLY	8.1
1	A	151	ALA	8.0
1	A	214	LEU	8.0
1	A	58	ASP	8.0
1	A	174	CYS	7.8
1	A	49	ILE	7.8
1	A	26	MET	7.7
1	A	216	ASN	7.7
1	A	139	LEU	7.7
1	A	322	ALA	7.7
1	A	109	MET	7.6
1	A	302	PHE	7.6
1	A	110	ASN	7.6
1	A	36	SER	7.5
1	A	115	LYS	7.5
1	A	83	GLU	7.4
1	A	262	LEU	7.4
1	A	133	GLY	7.4
1	A	150	VAL	7.3
1	A	23	ARG	7.2
1	A	153	PHE	7.2
1	A	64	ALA	7.1
1	A	267	LEU	7.1
1	A	70	ALA	7.1
1	A	265	GLU	7.0
1	A	306	PRO	7.0
1	A	278	LYS	7.0
1	A	4	LYS	7.0
1	A	15	GLU	6.9
1	A	293	LEU	6.8
1	A	95	TYR	6.8
1	A	152	ASN	6.7
1	A	320	VAL	6.7
1	A	232	ARG	6.7
1	A	105	SER	6.7
1	A	54	ALA	6.7
1	A	188	TYR	6.6
1	A	161	CYS	6.6
1	A	114	GLY	6.6
1	A	11	VAL	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	86	GLY	6.5
1	A	260	GLU	6.5
1	A	143	ARG	6.4
1	A	124	ARG	6.4
1	A	291	LYS	6.4
1	A	53	ALA	6.3
1	A	246	VAL	6.3
1	A	301	GLY	6.3
1	A	78	LYS	6.3
1	A	20	GLN	6.3
1	A	218	ALA	6.2
1	A	318	GLU	6.2
1	A	207	GLU	6.1
1	A	311	ALA	6.1
1	A	247	PRO	6.1
1	A	126	ALA	6.0
1	A	212	GLU	6.0
1	A	120	THR	6.0
1	A	266	LEU	6.0
1	A	316	GLY	6.0
1	A	123	GLY	5.9
1	A	59	ALA	5.9
1	A	223	TYR	5.9
1	A	27	LYS	5.8
1	A	314	TYR	5.8
1	A	319	TYR	5.7
1	A	130	ILE	5.7
1	A	186	PHE	5.6
1	A	254	ARG	5.6
1	A	327	ARG	5.6
1	A	57	ALA	5.5
1	A	45	TYR	5.4
1	A	298	SER	5.4
1	A	307	PRO	5.4
1	A	315	LEU	5.4
1	A	184	GLN	5.4
1	A	119	HIS	5.4
1	A	149	ALA	5.3
1	A	286	SER	5.3
1	A	251	VAL	5.3
1	A	252	VAL	5.2
1	A	279	SER	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	102	LYS	5.1
1	A	65	GLY	5.1
1	A	111	GLN	5.0
1	A	146	LEU	5.0
1	A	250	THR	4.9
1	A	290	GLY	4.9
1	A	107	PHE	4.8
1	A	66	LEU	4.8
1	A	292	ASP	4.8
1	A	21	SER	4.8
1	A	10	ALA	4.7
1	A	248	SER	4.7
1	A	104	ASP	4.6
1	A	44	SER	4.6
1	A	321	THR	4.6
1	A	162	ALA	4.5
1	A	122	LEU	4.5
1	A	224	GLU	4.5
1	A	140	PRO	4.4
1	A	69	ASP	4.4
1	A	296	LYS	4.3
1	A	121	GLY	4.3
1	A	155	SER	4.3
1	A	29	VAL	4.2
1	A	79	PRO	4.2
1	A	142	PRO	4.2
1	A	97	ALA	4.2
1	A	158	CYS	4.2
1	A	60	VAL	4.2
1	A	253	ALA	4.1
1	A	99	ALA	4.0
1	A	145	PRO	4.0
1	A	18	LYS	3.9
1	A	160	PRO	3.9
1	A	245	GLN	3.8
1	A	180	SER	3.7
1	A	148	LYS	3.5
1	A	108	GLN	3.3
1	A	297	ASP	3.3
1	A	144	LYS	3.1
1	A	220	ARG	3.1
1	A	187	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	273	HIS	3.1
1	A	270	ALA	3.0
1	A	269	GLN	2.9
1	A	221	ASP	2.7
1	A	217	LYS	2.5
1	A	268	ASN	2.4
1	A	272	GLU	2.4

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CO3	A	338	4/4	-0.23	0.53	-0.46	11,13,16,17	0
3	FE	A	339	1/1	-0.41	0.43	-1.07	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.