



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:17 AM GMT

PDB ID : 1D3K  
Title : HUMAN SERUM TRANSFERRIN  
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Deposited on : 1999-09-29  
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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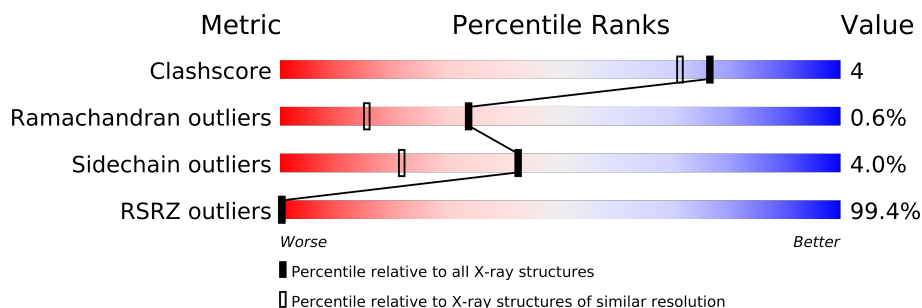
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	329	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CO3	A	338	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 2695 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

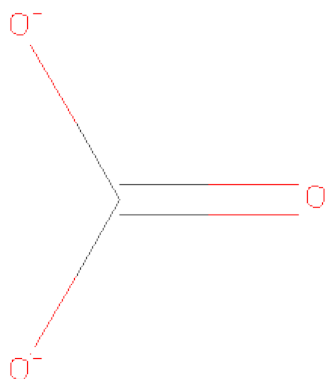
- Molecule 1 is a protein called SERUM TRANSFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	329	2551	1611	437	482	21	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	GLN	LYS	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

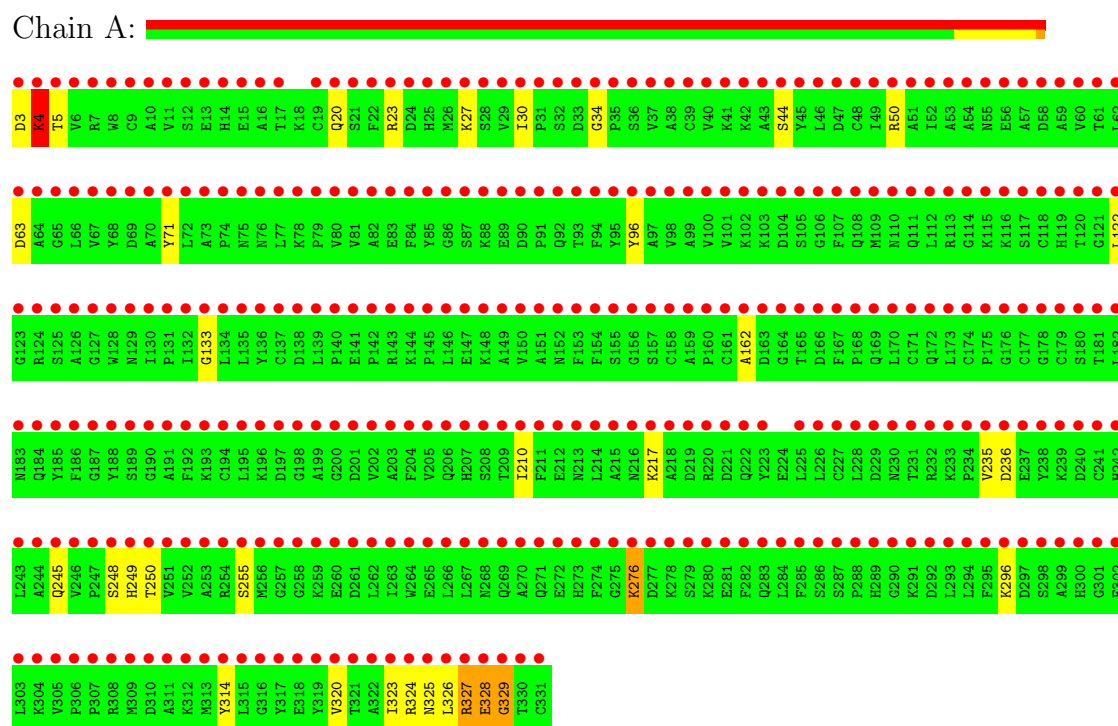
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total 139	O 139	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: SERUM TRANSFERRIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.01Å 57.81Å 135.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 1.80 34.36 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-1.80) 91.0 (34.36-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.57 (at 1.81Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.184 , 0.225 0.193 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30614 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.43	0/2612	0.65	1/3531 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	5	THR	N-CA-C	5.09	124.73	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2551	0	2462	19	0
2	A	4	0	0	0	0
3	A	1	0	0	0	0
4	A	139	0	0	2	0
All	All	2695	0	2462	19	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (19) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:3:ASP:O	1:A:4:LYS:HB2	1.82	0.78
1:A:250:THR:HG21	1:A:314:TYR:CZ	2.30	0.67
1:A:250:THR:HG21	1:A:314:TYR:CE2	2.30	0.67
1:A:325:ASN:O	1:A:329:GLY:HA3	2.00	0.61
1:A:30:ILE:CG2	1:A:34:GLY:HA3	2.32	0.59
1:A:96:TYR:HE1	1:A:245:GLN:HE21	1.53	0.56
1:A:276:LYS:HE2	4:A:443:HOH:O	2.04	0.56
1:A:63:ASP:HA	1:A:249:HIS:CD2	2.46	0.51
1:A:23:ARG:HG2	1:A:27:LYS:HE3	1.92	0.51
1:A:122:LEU:HD22	1:A:162:ALA:HA	1.96	0.48
1:A:323:ILE:O	1:A:327:ARG:HD2	2.14	0.47
1:A:249:HIS:CE1	1:A:296:LYS:HD2	2.54	0.43
1:A:30:ILE:HG23	1:A:34:GLY:HA3	1.99	0.41
1:A:50:ARG:HG3	4:A:467:HOH:O	2.20	0.41
1:A:328:GLU:O	1:A:329:GLY:O	2.39	0.41
1:A:320:VAL:O	1:A:324:ARG:HG3	2.21	0.41
1:A:250:THR:CG2	1:A:314:TYR:OH	2.69	0.41
1:A:210:ILE:HD13	1:A:235:VAL:HG11	2.04	0.40
1:A:133:GLY:HA2	1:A:326:LEU:HD13	2.04	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%)	311 (95%)	14 (4%)	2 (1%)	33	15

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%)	263 (96%)	11 (4%)	42 22

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	20	GLN
1	A	44	SER
1	A	71	TYR
1	A	217	LYS
1	A	236	ASP
1	A	248	SER
1	A	255	SER
1	A	276	LYS
1	A	327	ARG
1	A	328	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

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

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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%)	7.43	327 (99%) 0 0	14, 24, 56, 84	4 (1%)

All (327) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	ASP	29.0
1	A	211	PHE	26.4
1	A	106	GLY	26.0
1	A	231	THR	21.8
1	A	30	ILE	20.1
1	A	230	ASN	19.4
1	A	247	PRO	19.2
1	A	205	VAL	18.7
1	A	330	THR	18.5
1	A	87	SER	17.9
1	A	258	GLY	17.4
1	A	257	GLY	17.3
1	A	29	VAL	16.5
1	A	163	ASP	16.0
1	A	144	LYS	15.9
1	A	317	TYR	15.8
1	A	244	ALA	15.6
1	A	167	PHE	15.5
1	A	140	PRO	15.2
1	A	234	PRO	15.2
1	A	168	PRO	15.1
1	A	5	THR	14.6
1	A	137	CYS	14.6
1	A	38	ALA	14.4
1	A	81	VAL	14.4
1	A	165	THR	14.1
1	A	71	TYR	14.1

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Mol	Chain	Res	Type	RSRZ
1	A	68	TYR	14.0
1	A	135	LEU	13.9
1	A	113	ARG	13.9
1	A	328	GLU	13.6
1	A	33	ASP	13.4
1	A	61	THR	13.3
1	A	157	SER	13.2
1	A	109	MET	13.1
1	A	154	PHE	13.1
1	A	331	CYS	13.0
1	A	324	ARG	13.0
1	A	178	GLY	12.9
1	A	65	GLY	12.7
1	A	263	ILE	12.6
1	A	117	SER	12.6
1	A	228	LEU	12.5
1	A	3	ASP	12.5
1	A	209	THR	12.4
1	A	196	LYS	12.1
1	A	255	SER	12.0
1	A	73	ALA	12.0
1	A	35	PRO	12.0
1	A	134	LEU	11.7
1	A	236	ASP	11.4
1	A	90	ASP	11.3
1	A	325	ASN	11.2
1	A	274	PHE	11.1
1	A	43	ALA	11.0
1	A	280	LYS	10.7
1	A	329	GLY	10.7
1	A	152	ASN	10.6
1	A	237	GLU	10.6
1	A	308	ARG	10.5
1	A	264	TRP	10.4
1	A	63	ASP	10.3
1	A	50	ARG	10.3
1	A	110	ASN	10.3
1	A	189	SER	10.2
1	A	316	GLY	10.2
1	A	12	SER	10.2
1	A	32	SER	10.1
1	A	215	ALA	10.0

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Mol	Chain	Res	Type	RSRZ
1	A	208	SER	9.8
1	A	22	PHE	9.8
1	A	139	LEU	9.8
1	A	6	VAL	9.8
1	A	52	ILE	9.6
1	A	210	ILE	9.6
1	A	239	LYS	9.5
1	A	273	HIS	9.4
1	A	69	ASP	9.3
1	A	232	ARG	9.3
1	A	259	LYS	9.3
1	A	7	ARG	9.2
1	A	141	GLU	9.0
1	A	89	GLU	8.9
1	A	222	GLN	8.7
1	A	300	HIS	8.7
1	A	128	TRP	8.6
1	A	194	CYS	8.6
1	A	130	ILE	8.6
1	A	24	ASP	8.5
1	A	305	VAL	8.5
1	A	17	THR	8.5
1	A	77	LEU	8.3
1	A	302	PHE	8.3
1	A	95	TYR	8.3
1	A	96	TYR	8.2
1	A	136	TYR	8.2
1	A	100	VAL	8.2
1	A	28	SER	8.1
1	A	261	ASP	8.0
1	A	288	PRO	8.0
1	A	51	ALA	7.9
1	A	20	GLN	7.9
1	A	206	GLN	7.9
1	A	246	VAL	7.9
1	A	248	SER	7.8
1	A	19	CYS	7.8
1	A	191	ALA	7.7
1	A	278	LYS	7.6
1	A	16	ALA	7.6
1	A	277	ASP	7.6
1	A	282	PHE	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	176	GLY	7.6
1	A	31	PRO	7.6
1	A	67	VAL	7.6
1	A	75	ASN	7.6
1	A	72	LEU	7.6
1	A	74	PRO	7.5
1	A	127	GLY	7.5
1	A	193	LYS	7.5
1	A	323	ILE	7.5
1	A	238	TYR	7.5
1	A	314	TYR	7.4
1	A	98	VAL	7.3
1	A	241	CYS	7.3
1	A	49	ILE	7.3
1	A	34	GLY	7.2
1	A	93	THR	7.2
1	A	186	PHE	7.2
1	A	326	LEU	7.1
1	A	4	LYS	7.1
1	A	56	GLU	7.1
1	A	240	ASP	7.1
1	A	94	PHE	7.0
1	A	39	CYS	7.0
1	A	25	HIS	7.0
1	A	283	GLN	7.0
1	A	45	TYR	7.0
1	A	181	THR	6.9
1	A	170	LEU	6.9
1	A	214	LEU	6.9
1	A	125	SER	6.8
1	A	233	LYS	6.8
1	A	13	GLU	6.8
1	A	86	GLY	6.8
1	A	126	ALA	6.7
1	A	104	ASP	6.7
1	A	21	SER	6.7
1	A	150	VAL	6.7
1	A	120	THR	6.7
1	A	82	ALA	6.7
1	A	8	TRP	6.6
1	A	309	MET	6.6
1	A	62	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	312	LYS	6.6
1	A	195	LEU	6.6
1	A	147	GLU	6.5
1	A	116	LYS	6.5
1	A	97	ALA	6.5
1	A	118	CYS	6.5
1	A	58	ASP	6.4
1	A	262	LEU	6.4
1	A	23	ARG	6.4
1	A	265	GLU	6.4
1	A	88	LYS	6.4
1	A	291	LYS	6.4
1	A	64	ALA	6.3
1	A	153	PHE	6.2
1	A	129	ASN	6.2
1	A	91	PRO	6.2
1	A	188	TYR	6.2
1	A	166	ASP	6.2
1	A	183	ASN	6.2
1	A	40	VAL	6.1
1	A	227	CYS	6.1
1	A	84	PHE	6.1
1	A	304	LYS	6.1
1	A	36	SER	6.1
1	A	133	GLY	6.1
1	A	310	ASP	6.0
1	A	321	THR	6.0
1	A	173	LEU	6.0
1	A	299	ALA	6.0
1	A	53	ALA	6.0
1	A	285	PHE	5.9
1	A	281	GLU	5.9
1	A	190	GLY	5.9
1	A	204	PHE	5.8
1	A	320	VAL	5.8
1	A	171	CYS	5.7
1	A	164	GLY	5.7
1	A	59	ALA	5.7
1	A	138	ASP	5.6
1	A	27	LYS	5.6
1	A	212	GLU	5.6
1	A	250	THR	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	256	MET	5.6
1	A	319	TYR	5.6
1	A	114	GLY	5.6
1	A	295	PHE	5.6
1	A	251	VAL	5.6
1	A	192	PHE	5.6
1	A	123	GLY	5.6
1	A	269	GLN	5.5
1	A	198	GLY	5.5
1	A	99	ALA	5.5
1	A	184	GLN	5.5
1	A	284	LEU	5.4
1	A	185	TYR	5.4
1	A	42	LYS	5.4
1	A	76	ASN	5.4
1	A	143	ARG	5.3
1	A	80	VAL	5.3
1	A	156	GLY	5.3
1	A	200	GLY	5.3
1	A	131	PRO	5.3
1	A	322	ALA	5.2
1	A	107	PHE	5.2
1	A	182	LEU	5.2
1	A	294	LEU	5.1
1	A	318	GLU	5.1
1	A	57	ALA	5.1
1	A	112	LEU	5.1
1	A	161	CYS	5.1
1	A	103	LYS	5.0
1	A	92	GLN	5.0
1	A	14	HIS	5.0
1	A	145	PRO	5.0
1	A	46	LEU	5.0
1	A	70	ALA	4.9
1	A	223	TYR	4.9
1	A	311	ALA	4.9
1	A	146	LEU	4.9
1	A	301	GLY	4.8
1	A	132	ILE	4.8
1	A	54	ALA	4.8
1	A	41	LYS	4.8
1	A	26	MET	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	155	SER	4.8
1	A	78	LYS	4.8
1	A	268	ASN	4.8
1	A	235	VAL	4.8
1	A	221	ASP	4.7
1	A	111	GLN	4.7
1	A	218	ALA	4.7
1	A	148	LYS	4.7
1	A	293	LEU	4.7
1	A	174	CYS	4.7
1	A	172	GLN	4.6
1	A	266	LEU	4.6
1	A	177	CYS	4.6
1	A	216	ASN	4.6
1	A	162	ALA	4.5
1	A	11	VAL	4.5
1	A	260	GLU	4.5
1	A	44	SER	4.4
1	A	124	ARG	4.3
1	A	202	VAL	4.3
1	A	315	LEU	4.3
1	A	313	MET	4.3
1	A	296	LYS	4.2
1	A	243	LEU	4.2
1	A	37	VAL	4.2
1	A	249	HIS	4.2
1	A	179	CYS	4.2
1	A	48	CYS	4.2
1	A	169	GLN	4.2
1	A	267	LEU	4.2
1	A	101	VAL	4.1
1	A	213	ASN	4.1
1	A	226	LEU	3.9
1	A	160	PRO	3.8
1	A	245	GLN	3.8
1	A	197	ASP	3.8
1	A	289	HIS	3.7
1	A	108	GLN	3.7
1	A	286	SER	3.7
1	A	187	GLY	3.7
1	A	158	CYS	3.7
1	A	225	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	122	LEU	3.6
1	A	303	LEU	3.6
1	A	290	GLY	3.6
1	A	297	ASP	3.6
1	A	66	LEU	3.6
1	A	142	PRO	3.6
1	A	119	HIS	3.6
1	A	272	GLU	3.6
1	A	9	CYS	3.6
1	A	47	ASP	3.6
1	A	327	ARG	3.5
1	A	217	LYS	3.5
1	A	85	TYR	3.5
1	A	60	VAL	3.5
1	A	10	ALA	3.5
1	A	115	LYS	3.5
1	A	201	ASP	3.5
1	A	180	SER	3.4
1	A	254	ARG	3.4
1	A	219	ASP	3.4
1	A	79	PRO	3.4
1	A	287	SER	3.4
1	A	175	PRO	3.3
1	A	279	SER	3.3
1	A	252	VAL	3.3
1	A	149	ALA	3.3
1	A	203	ALA	3.3
1	A	220	ARG	3.3
1	A	102	LYS	3.2
1	A	292	ASP	3.2
1	A	242	HIS	3.2
1	A	105	SER	3.2
1	A	307	PRO	3.2
1	A	276	LYS	3.1
1	A	271	GLN	3.1
1	A	270	ALA	3.0
1	A	159	ALA	3.0
1	A	83	GLU	2.8
1	A	298	SER	2.7
1	A	151	ALA	2.7
1	A	306	PRO	2.6
1	A	55	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	253	ALA	2.5
1	A	15	GLU	2.5
1	A	275	GLY	2.2
1	A	121	GLY	2.1
1	A	207	HIS	2.1
1	A	199	ALA	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CO3	A	338	4/4	1.05	4.44	15,17,17,18	0
3	FE	A	339	1/1	0.42	-0.60	15,15,15,15	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.