



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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

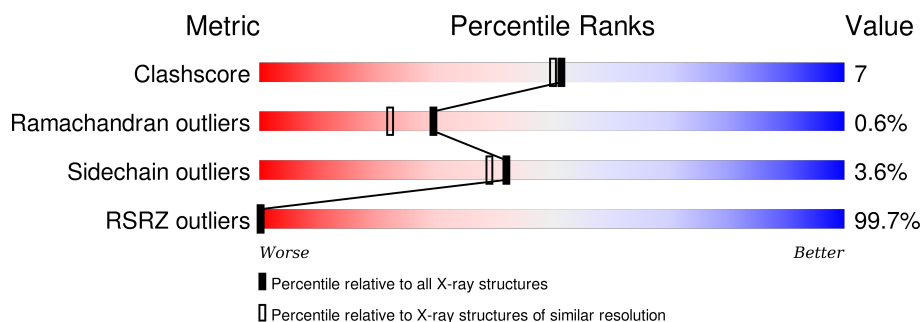
1 Overall quality at a glance

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 ≥ 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>

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.

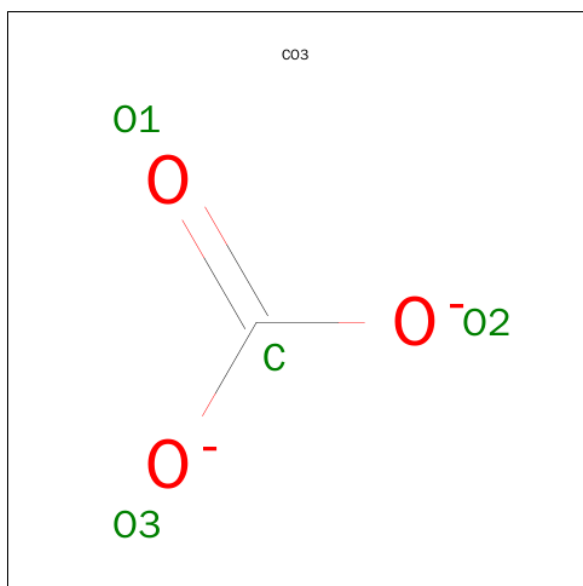
- Molecule 1 is a protein called TRANSFERRIN.

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: CO₃).



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

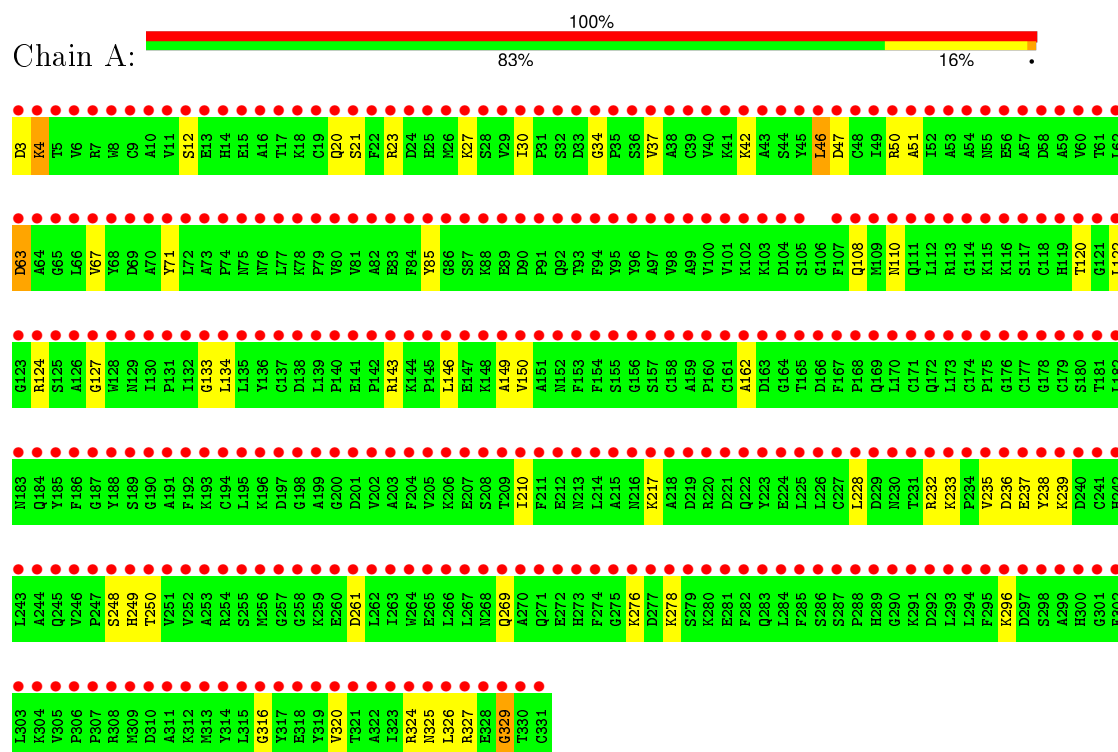
- Molecule 4 is water.

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

3 Residue-property plots

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 ($RSRZ > 2$). 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, α , β , γ	45.03 Å 57.91 Å 135.90 Å 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
$\langle I/\sigma(I) \rangle$ ¹	0.59 (at 2.00 Å)	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 ²)	21.5	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 21716 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2690	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:85:TYR:CE2	1:A:248:SER:HB3	2.45	0.51
1:A:23:ARG:HG3	1:A:37:VAL:O	2.11	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:42:LYS:HD2	1:A:47:ASP:HB3	2.00	0.44
1:A:233:LYS:HD3	1:A:237:GLU:OE1	2.17	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%)	30	22

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%)	42	39

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, 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	329/329 (100%)	12.35	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	45.9
1	A	284	LEU	43.9
1	A	282	PHE	39.1
1	A	209	THR	39.0
1	A	192	PHE	38.9
1	A	330	THR	37.1
1	A	229	ASP	36.9
1	A	200	GLY	35.5
1	A	182	LEU	33.8
1	A	205	VAL	32.6
1	A	303	LEU	32.5
1	A	228	LEU	32.4
1	A	135	LEU	31.2
1	A	171	CYS	30.2
1	A	73	ALA	28.6
1	A	210	ILE	28.3
1	A	43	ALA	27.7
1	A	178	GLY	27.4
1	A	283	GLN	27.4
1	A	75	ASN	27.3
1	A	137	CYS	27.1
1	A	288	PRO	26.9
1	A	117	SER	26.2
1	A	309	MET	26.0
1	A	40	VAL	25.9
1	A	213	ASN	25.9
1	A	199	ALA	25.5

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Mol	Chain	Res	Type	RSRZ
1	A	194	CYS	25.3
1	A	91	PRO	24.7
1	A	166	ASP	24.2
1	A	263	ILE	24.1
1	A	90	ASP	23.7
1	A	98	VAL	23.3
1	A	128	TRP	23.2
1	A	211	PHE	22.8
1	A	89	GLU	22.3
1	A	227	CYS	22.2
1	A	87	SER	22.2
1	A	308	ARG	22.1
1	A	304	LYS	21.6
1	A	84	PHE	21.4
1	A	203	ALA	21.2
1	A	237	GLU	21.2
1	A	233	LYS	20.7
1	A	275	GLY	20.6
1	A	305	VAL	20.5
1	A	52	ILE	20.0
1	A	195	LEU	20.0
1	A	35	PRO	19.8
1	A	202	VAL	19.4
1	A	138	ASP	19.3
1	A	163	ASP	19.1
1	A	236	ASP	19.1
1	A	136	TYR	19.0
1	A	22	PHE	19.0
1	A	34	GLY	18.6
1	A	5	THR	18.5
1	A	134	LEU	18.4
1	A	300	HIS	18.3
1	A	242	HIS	18.3
1	A	131	PRO	18.3
1	A	31	PRO	18.2
1	A	165	THR	18.2
1	A	81	VAL	18.2
1	A	240	ASP	18.2
1	A	310	ASP	18.0
1	A	239	LYS	18.0
1	A	38	ALA	18.0
1	A	16	ALA	17.7

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Mol	Chain	Res	Type	RSRZ
1	A	201	ASP	17.7
1	A	329	GLY	17.4
1	A	234	PRO	17.4
1	A	259	LYS	17.4
1	A	177	CYS	17.4
1	A	42	LYS	17.1
1	A	274	PHE	16.8
1	A	7	ARG	16.7
1	A	231	THR	16.7
1	A	173	LEU	16.6
1	A	68	TYR	16.3
1	A	6	VAL	16.3
1	A	243	LEU	16.2
1	A	3	ASP	16.1
1	A	331	CYS	16.1
1	A	197	ASP	15.9
1	A	72	LEU	15.9
1	A	196	LYS	15.9
1	A	51	ALA	15.9
1	A	46	LEU	15.4
1	A	71	TYR	15.3
1	A	37	VAL	15.3
1	A	198	GLY	15.3
1	A	255	SER	15.0
1	A	61	THR	15.0
1	A	76	ASN	14.9
1	A	193	LYS	14.8
1	A	206	LYS	14.6
1	A	172	GLN	14.6
1	A	156	GLY	14.6
1	A	328	GLU	14.5
1	A	287	SER	14.5
1	A	113	ARG	14.4
1	A	32	SER	14.4
1	A	169	GLN	14.2
1	A	295	PHE	14.1
1	A	168	PRO	14.1
1	A	183	ASN	14.1
1	A	244	ALA	14.0
1	A	170	LEU	13.9
1	A	324	ARG	13.8
1	A	176	GLY	13.7

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Mol	Chain	Res	Type	RSRZ
1	A	56	GLU	13.7
1	A	175	PRO	13.6
1	A	141	GLU	13.6
1	A	47	ASP	13.5
1	A	289	HIS	13.3
1	A	157	SER	13.2
1	A	312	LYS	13.1
1	A	39	CYS	12.9
1	A	25	HIS	12.7
1	A	179	CYS	12.7
1	A	285	PHE	12.7
1	A	77	LEU	12.7
1	A	238	TYR	12.7
1	A	55	ASN	12.6
1	A	127	GLY	12.4
1	A	294	LEU	12.4
1	A	96	TYR	12.4
1	A	276	LYS	12.4
1	A	24	ASP	12.4
1	A	181	THR	12.1
1	A	280	LYS	12.1
1	A	8	TRP	12.1
1	A	326	LEU	12.1
1	A	261	ASP	12.0
1	A	74	PRO	12.0
1	A	88	LYS	11.9
1	A	154	PHE	11.8
1	A	317	TYR	11.7
1	A	41	LYS	11.6
1	A	129	ASN	11.6
1	A	82	ALA	11.4
1	A	167	PHE	11.2
1	A	313	MET	11.1
1	A	277	ASP	11.0
1	A	185	TYR	11.0
1	A	264	TRP	11.0
1	A	204	PHE	11.0
1	A	30	ILE	11.0
1	A	125	SER	10.9
1	A	191	ALA	10.9
1	A	112	LEU	10.9
1	A	100	VAL	10.9

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Mol	Chain	Res	Type	RSRZ
1	A	118	CYS	10.8
1	A	33	ASP	10.8
1	A	257	GLY	10.8
1	A	164	GLY	10.7
1	A	94	PHE	10.7
1	A	12	SER	10.6
1	A	235	VAL	10.5
1	A	132	ILE	10.5
1	A	222	GLN	10.5
1	A	28	SER	10.4
1	A	17	THR	10.3
1	A	241	CYS	10.2
1	A	258	GLY	10.2
1	A	50	ARG	10.1
1	A	116	LYS	10.0
1	A	215	ALA	10.0
1	A	225	LEU	10.0
1	A	80	VAL	9.9
1	A	67	VAL	9.8
1	A	14	HIS	9.8
1	A	208	SER	9.8
1	A	19	CYS	9.6
1	A	103	LYS	9.6
1	A	48	CYS	9.5
1	A	189	SER	9.5
1	A	85	TYR	9.4
1	A	219	ASP	9.4
1	A	271	GLN	9.3
1	A	101	VAL	9.2
1	A	325	ASN	9.0
1	A	323	ILE	8.9
1	A	147	GLU	8.9
1	A	299	ALA	8.8
1	A	62	LEU	8.8
1	A	63	ASP	8.7
1	A	226	LEU	8.7
1	A	93	THR	8.6
1	A	92	GLN	8.6
1	A	159	ALA	8.5
1	A	13	GLU	8.5
1	A	9	CYS	8.5
1	A	151	ALA	8.5

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Mol	Chain	Res	Type	RSRZ
1	A	190	GLY	8.4
1	A	281	GLU	8.4
1	A	214	LEU	8.4
1	A	249	HIS	8.3
1	A	58	ASP	8.3
1	A	256	MET	8.3
1	A	49	ILE	8.2
1	A	174	CYS	8.1
1	A	139	LEU	8.0
1	A	322	ALA	8.0
1	A	302	PHE	8.0
1	A	216	ASN	7.9
1	A	26	MET	7.9
1	A	110	ASN	7.8
1	A	36	SER	7.8
1	A	109	MET	7.8
1	A	262	LEU	7.7
1	A	150	VAL	7.7
1	A	133	GLY	7.7
1	A	115	LYS	7.7
1	A	83	GLU	7.6
1	A	153	PHE	7.5
1	A	64	ALA	7.5
1	A	23	ARG	7.4
1	A	70	ALA	7.4
1	A	267	LEU	7.4
1	A	306	PRO	7.3
1	A	265	GLU	7.2
1	A	4	LYS	7.2
1	A	278	LYS	7.2
1	A	320	VAL	7.2
1	A	293	LEU	7.1
1	A	15	GLU	7.1
1	A	11	VAL	7.0
1	A	54	ALA	7.0
1	A	95	TYR	7.0
1	A	105	SER	7.0
1	A	152	ASN	6.9
1	A	114	GLY	6.9
1	A	232	ARG	6.9
1	A	161	CYS	6.9
1	A	188	TYR	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	86	GLY	6.8
1	A	246	VAL	6.8
1	A	260	GLU	6.7
1	A	53	ALA	6.7
1	A	301	GLY	6.6
1	A	124	ARG	6.6
1	A	143	ARG	6.6
1	A	218	ALA	6.6
1	A	291	LYS	6.6
1	A	78	LYS	6.5
1	A	20	GLN	6.5
1	A	311	ALA	6.4
1	A	126	ALA	6.4
1	A	318	GLU	6.4
1	A	247	PRO	6.3
1	A	266	LEU	6.3
1	A	207	GLU	6.3
1	A	316	GLY	6.2
1	A	59	ALA	6.2
1	A	120	THR	6.2
1	A	123	GLY	6.2
1	A	212	GLU	6.2
1	A	223	TYR	6.1
1	A	130	ILE	6.0
1	A	27	LYS	6.0
1	A	314	TYR	6.0
1	A	319	TYR	5.9
1	A	186	PHE	5.9
1	A	57	ALA	5.8
1	A	254	ARG	5.8
1	A	327	ARG	5.8
1	A	315	LEU	5.7
1	A	298	SER	5.6
1	A	149	ALA	5.6
1	A	307	PRO	5.6
1	A	45	TYR	5.6
1	A	251	VAL	5.6
1	A	252	VAL	5.6
1	A	184	GLN	5.5
1	A	119	HIS	5.5
1	A	286	SER	5.5
1	A	279	SER	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	65	GLY	5.4
1	A	102	LYS	5.3
1	A	146	LEU	5.3
1	A	111	GLN	5.2
1	A	107	PHE	5.1
1	A	290	GLY	5.1
1	A	66	LEU	5.1
1	A	250	THR	5.1
1	A	292	ASP	5.0
1	A	10	ALA	5.0
1	A	21	SER	4.9
1	A	248	SER	4.9
1	A	321	THR	4.8
1	A	104	ASP	4.8
1	A	44	SER	4.8
1	A	162	ALA	4.8
1	A	122	LEU	4.7
1	A	140	PRO	4.6
1	A	69	ASP	4.6
1	A	224	GLU	4.6
1	A	29	VAL	4.5
1	A	121	GLY	4.5
1	A	155	SER	4.5
1	A	97	ALA	4.4
1	A	60	VAL	4.4
1	A	296	LYS	4.4
1	A	79	PRO	4.4
1	A	142	PRO	4.4
1	A	158	CYS	4.4
1	A	253	ALA	4.3
1	A	99	ALA	4.2
1	A	145	PRO	4.1
1	A	18	LYS	4.1
1	A	160	PRO	4.0
1	A	245	GLN	3.9
1	A	180	SER	3.9
1	A	148	LYS	3.6
1	A	108	GLN	3.5
1	A	297	ASP	3.4
1	A	144	LYS	3.2
1	A	187	GLY	3.2
1	A	220	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	273	HIS	3.2
1	A	270	ALA	3.2
1	A	269	GLN	3.0
1	A	221	ASP	2.8
1	A	217	LYS	2.6
1	A	268	ASN	2.5
1	A	272	GLU	2.5

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, 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	LLDF	B-factors(\AA^2)	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	-1.08	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.