



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 02:18 PM EDT

PDB ID : 1D3K
Title : HUMAN SERUM TRANSFERRIN
Authors : Yang, H.-W.; MacGillivray, R.T.A.; Chen, J.; Luo, Y.; Wang, Y.; Brayer, G.D.; Mason, A.; Woodworth, R.C.; Murphy, M.E.P.
Deposited on : 1999-09-29
Resolution : 1.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

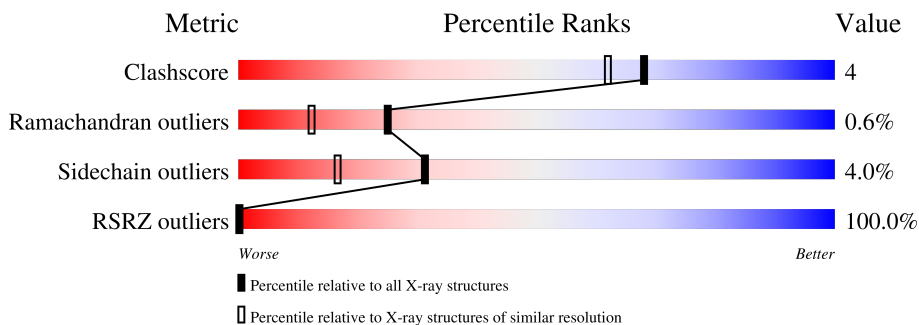
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 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	329	

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 2695 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.

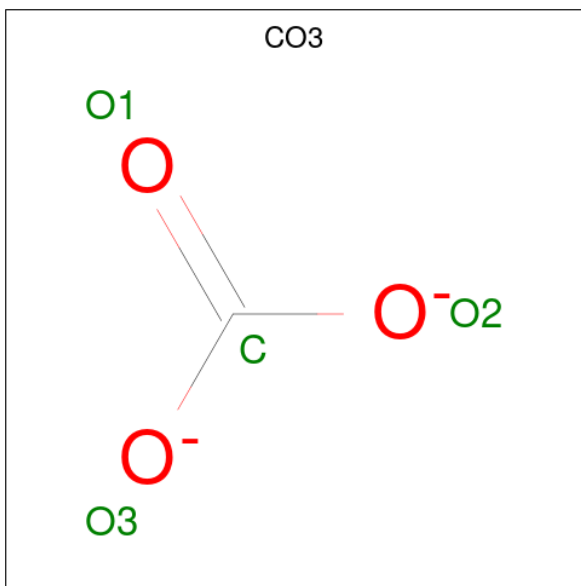
- Molecule 1 is a protein called SERUM TRANSFERRIN.

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 mutation	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	Fe	0	0
			1	1		

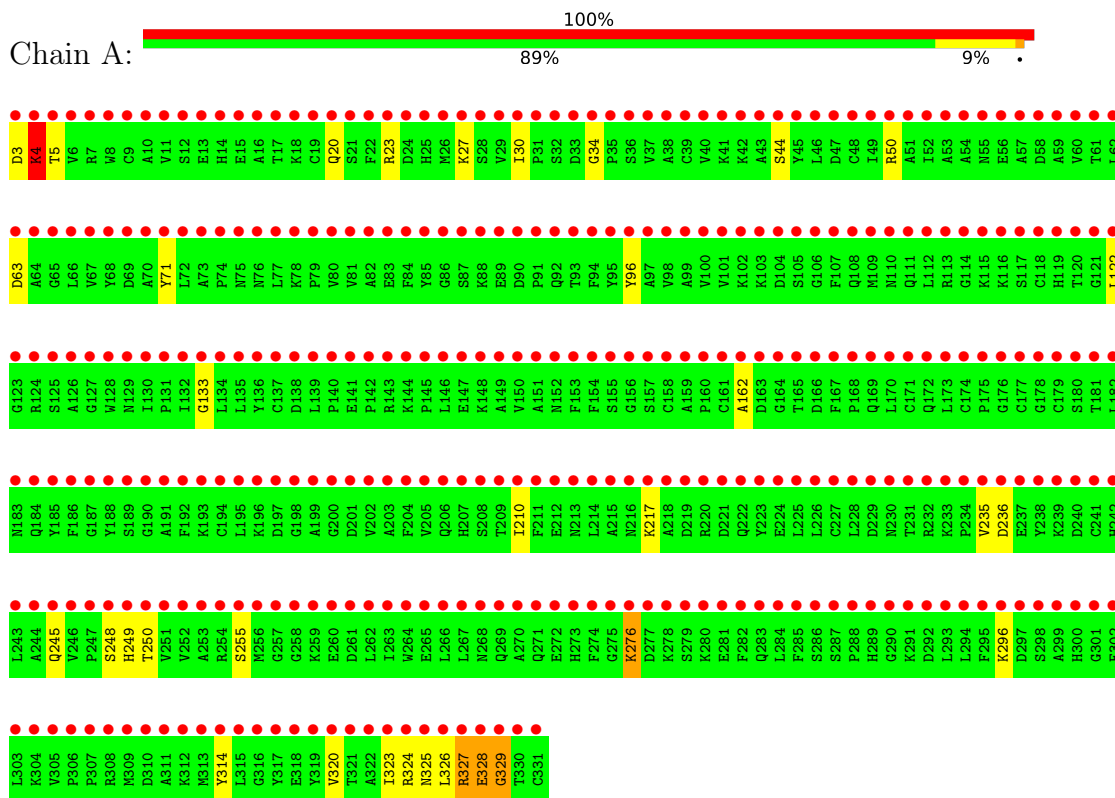
- Molecule 4 is water.

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

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: SERUM TRANSFERRIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.01Å 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
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 1.81Å)	Xtrriage
Refinement program	XTALVIEW, X-PLOR 3.851	Depositor
R, R_{free}	0.184 , 0.225 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtrriage
Anisotropy	0.188	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2695	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage'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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, CO3

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(°)	Ideal(°)
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 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	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

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 4.

All (19) 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	0.78
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:320:VAL:O	1:A:324:ARG:HG3	2.21	0.41
1:A:328:GLU:O	1:A:329:GLY:O	2.39	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 [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	327/329 (99%)	311 (95%)	14 (4%)	2 (1%)	25 12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS

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Mol	Chain	Res	Type
1	A	329	GLY

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	274/274 (100%)	263 (96%)	11 (4%)	31 16

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

Sometimes 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 [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 monosaccharides 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	-	-	0,3,3	-	-

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	329/329 (100%)	8.42	329 (100%) 0 0	14, 24, 56, 84	4 (1%)

All (329) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	PHE	24.8
1	A	211	PHE	22.6
1	A	68	TYR	22.3
1	A	106	GLY	20.7
1	A	329	GLY	20.5
1	A	3	ASP	20.0
1	A	247	PRO	19.8
1	A	29	VAL	18.3
1	A	33	ASP	18.2
1	A	229	ASP	17.8
1	A	205	VAL	17.2
1	A	330	THR	17.1
1	A	274	PHE	16.7
1	A	331	CYS	16.6
1	A	317	TYR	16.5
1	A	30	ILE	16.3
1	A	222	GLN	15.8
1	A	328	GLU	15.6
1	A	255	SER	14.6
1	A	191	ALA	14.5
1	A	154	PHE	14.5
1	A	128	TRP	14.4
1	A	326	LEU	14.0
1	A	248	SER	13.8
1	A	87	SER	13.7
1	A	100	VAL	13.6
1	A	61	THR	13.3

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Mol	Chain	Res	Type	RSRZ
1	A	50	ARG	13.1
1	A	258	GLY	13.1
1	A	264	TRP	13.1
1	A	231	THR	13.0
1	A	71	TYR	13.0
1	A	204	PHE	12.9
1	A	178	GLY	12.8
1	A	244	ALA	12.7
1	A	168	PRO	12.7
1	A	153	PHE	12.5
1	A	305	VAL	12.5
1	A	113	ARG	12.5
1	A	325	ASN	12.3
1	A	35	PRO	12.3
1	A	51	ALA	12.2
1	A	210	ILE	12.1
1	A	163	ASP	12.1
1	A	209	THR	12.0
1	A	186	PHE	12.0
1	A	324	ARG	12.0
1	A	165	THR	12.0
1	A	104	ASP	12.0
1	A	109	MET	11.9
1	A	32	SER	11.8
1	A	73	ALA	11.7
1	A	236	ASP	11.7
1	A	228	LEU	11.6
1	A	316	GLY	11.6
1	A	302	PHE	11.6
1	A	58	ASP	11.5
1	A	189	SER	11.5
1	A	277	ASP	11.5
1	A	196	LYS	11.5
1	A	117	SER	11.4
1	A	52	ILE	11.3
1	A	280	LYS	11.3
1	A	288	PRO	11.2
1	A	134	LEU	11.2
1	A	246	VAL	11.1
1	A	81	VAL	11.1
1	A	308	ARG	11.1
1	A	181	THR	11.0

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Mol	Chain	Res	Type	RSRZ
1	A	300	HIS	11.0
1	A	17	THR	11.0
1	A	314	TYR	10.9
1	A	69	ASP	10.8
1	A	144	LYS	10.8
1	A	96	TYR	10.8
1	A	5	THR	10.7
1	A	259	LYS	10.6
1	A	215	ALA	10.6
1	A	19	CYS	10.6
1	A	65	GLY	10.6
1	A	170	LEU	10.5
1	A	38	ALA	10.5
1	A	151	ALA	10.4
1	A	150	VAL	10.4
1	A	230	ASN	10.4
1	A	152	ASN	10.3
1	A	95	TYR	10.2
1	A	49	ILE	10.1
1	A	43	ALA	10.1
1	A	77	LEU	10.1
1	A	114	GLY	9.9
1	A	31	PRO	9.9
1	A	221	ASP	9.8
1	A	173	LEU	9.8
1	A	239	LYS	9.8
1	A	110	ASN	9.8
1	A	156	GLY	9.7
1	A	6	VAL	9.6
1	A	282	PHE	9.6
1	A	194	CYS	9.6
1	A	127	GLY	9.6
1	A	64	ALA	9.6
1	A	157	SER	9.6
1	A	67	VAL	9.5
1	A	321	THR	9.4
1	A	135	LEU	9.4
1	A	263	ILE	9.4
1	A	293	LEU	9.3
1	A	192	PHE	9.3
1	A	262	LEU	9.2
1	A	22	PHE	9.1

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Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	9.0
1	A	136	TYR	9.0
1	A	20	GLN	9.0
1	A	250	THR	8.9
1	A	285	PHE	8.9
1	A	90	ASP	8.9
1	A	202	VAL	8.8
1	A	237	GLU	8.8
1	A	24	ASP	8.8
1	A	234	PRO	8.7
1	A	34	GLY	8.6
1	A	88	LYS	8.6
1	A	241	CYS	8.6
1	A	232	ARG	8.6
1	A	123	GLY	8.5
1	A	75	ASN	8.5
1	A	98	VAL	8.5
1	A	12	SER	8.4
1	A	80	VAL	8.4
1	A	147	GLU	8.4
1	A	319	TYR	8.4
1	A	132	ILE	8.4
1	A	146	LEU	8.3
1	A	130	ILE	8.3
1	A	140	PRO	8.3
1	A	76	ASN	8.3
1	A	27	LYS	8.3
1	A	82	ALA	8.2
1	A	323	ILE	8.2
1	A	45	TYR	8.2
1	A	273	HIS	8.2
1	A	235	VAL	8.2
1	A	74	PRO	8.1
1	A	120	THR	8.1
1	A	93	THR	8.1
1	A	251	VAL	8.0
1	A	142	PRO	8.0
1	A	129	ASN	8.0
1	A	266	LEU	8.0
1	A	195	LEU	7.9
1	A	62	LEU	7.9
1	A	103	LYS	7.8

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Mol	Chain	Res	Type	RSRZ
1	A	84	PHE	7.8
1	A	182	LEU	7.8
1	A	214	LEU	7.8
1	A	101	VAL	7.8
1	A	261	ASP	7.7
1	A	238	TYR	7.7
1	A	217	LYS	7.7
1	A	118	CYS	7.7
1	A	137	CYS	7.7
1	A	199	ALA	7.6
1	A	240	ASP	7.6
1	A	177	CYS	7.6
1	A	322	ALA	7.6
1	A	160	PRO	7.6
1	A	53	ALA	7.5
1	A	301	GLY	7.5
1	A	131	PRO	7.5
1	A	8	TRP	7.5
1	A	169	GLN	7.4
1	A	14	HIS	7.4
1	A	46	LEU	7.4
1	A	125	SER	7.4
1	A	203	ALA	7.3
1	A	97	ALA	7.3
1	A	208	SER	7.3
1	A	107	PHE	7.3
1	A	176	GLY	7.3
1	A	162	ALA	7.3
1	A	206	GLN	7.2
1	A	249	HIS	7.2
1	A	89	GLU	7.2
1	A	25	HIS	7.2
1	A	166	ASP	7.2
1	A	39	CYS	7.2
1	A	66	LEU	7.1
1	A	48	CYS	7.1
1	A	179	CYS	7.1
1	A	13	GLU	7.1
1	A	315	LEU	7.1
1	A	36	SER	7.1
1	A	126	ALA	7.0
1	A	253	ALA	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	94	PHE	6.9
1	A	312	LYS	6.9
1	A	105	SER	6.9
1	A	37	VAL	6.9
1	A	78	LYS	6.8
1	A	28	SER	6.8
1	A	158	CYS	6.8
1	A	299	ALA	6.8
1	A	63	ASP	6.8
1	A	295	PHE	6.7
1	A	185	TYR	6.7
1	A	213	ASN	6.7
1	A	265	GLU	6.6
1	A	175	PRO	6.6
1	A	310	ASP	6.6
1	A	284	LEU	6.6
1	A	171	CYS	6.6
1	A	7	ARG	6.6
1	A	278	LYS	6.6
1	A	291	LYS	6.5
1	A	309	MET	6.5
1	A	72	LEU	6.5
1	A	243	LEU	6.5
1	A	256	MET	6.5
1	A	289	HIS	6.5
1	A	143	ARG	6.5
1	A	183	ASN	6.5
1	A	161	CYS	6.5
1	A	11	VAL	6.5
1	A	188	TYR	6.4
1	A	164	GLY	6.4
1	A	294	LEU	6.4
1	A	56	GLU	6.4
1	A	41	LYS	6.4
1	A	91	PRO	6.3
1	A	4	LYS	6.3
1	A	304	LYS	6.2
1	A	218	ALA	6.1
1	A	272	GLU	6.1
1	A	155	SER	6.1
1	A	21	SER	6.0
1	A	269	GLN	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	112	LEU	6.0
1	A	223	TYR	6.0
1	A	148	LYS	6.0
1	A	320	VAL	5.9
1	A	227	CYS	5.9
1	A	116	LYS	5.9
1	A	190	GLY	5.9
1	A	200	GLY	5.9
1	A	198	GLY	5.8
1	A	306	PRO	5.8
1	A	303	LEU	5.8
1	A	268	ASN	5.8
1	A	245	GLN	5.8
1	A	16	ALA	5.8
1	A	57	ALA	5.8
1	A	60	VAL	5.8
1	A	260	GLU	5.8
1	A	257	GLY	5.7
1	A	141	GLU	5.7
1	A	138	ASP	5.6
1	A	283	GLN	5.6
1	A	23	ARG	5.6
1	A	85	TYR	5.6
1	A	271	GLN	5.6
1	A	174	CYS	5.5
1	A	193	LYS	5.5
1	A	59	ALA	5.5
1	A	327	ARG	5.5
1	A	318	GLU	5.5
1	A	197	ASP	5.5
1	A	270	ALA	5.4
1	A	92	GLN	5.4
1	A	225	LEU	5.4
1	A	281	GLU	5.4
1	A	313	MET	5.3
1	A	9	CYS	5.3
1	A	115	LYS	5.3
1	A	145	PRO	5.2
1	A	86	GLY	5.2
1	A	267	LEU	5.2
1	A	286	SER	5.2
1	A	252	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	226	LEU	5.2
1	A	40	VAL	5.1
1	A	290	GLY	5.0
1	A	124	ARG	5.0
1	A	54	ALA	5.0
1	A	201	ASP	4.9
1	A	70	ALA	4.9
1	A	276	LYS	4.9
1	A	26	MET	4.9
1	A	122	LEU	4.8
1	A	292	ASP	4.8
1	A	311	ALA	4.8
1	A	159	ALA	4.7
1	A	10	ALA	4.7
1	A	42	LYS	4.6
1	A	187	GLY	4.6
1	A	99	ALA	4.6
1	A	111	GLN	4.6
1	A	184	GLN	4.5
1	A	172	GLN	4.4
1	A	216	ASN	4.4
1	A	275	GLY	4.4
1	A	119	HIS	4.3
1	A	242	HIS	4.3
1	A	220	ARG	4.2
1	A	219	ASP	4.1
1	A	102	LYS	4.1
1	A	254	ARG	4.1
1	A	224	GLU	4.1
1	A	83	GLU	4.0
1	A	287	SER	4.0
1	A	44	SER	4.0
1	A	149	ALA	3.9
1	A	296	LYS	3.8
1	A	233	LYS	3.8
1	A	297	ASP	3.8
1	A	180	SER	3.8
1	A	133	GLY	3.7
1	A	47	ASP	3.7
1	A	212	GLU	3.4
1	A	108	GLN	3.3
1	A	121	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	79	PRO	3.1
1	A	55	ASN	3.1
1	A	15	GLU	3.0
1	A	279	SER	3.0
1	A	207	HIS	3.0
1	A	307	PRO	2.9
1	A	298	SER	2.9
1	A	18	LYS	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 monosaccharides 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(Å ²)	Q<0.9
2	CO3	A	338	4/4	0.20	0.95	15,17,17,18	0
3	FE	A	339	1/1	0.73	0.50	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.