



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:23 am GMT

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

<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	:	1.7.2 (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

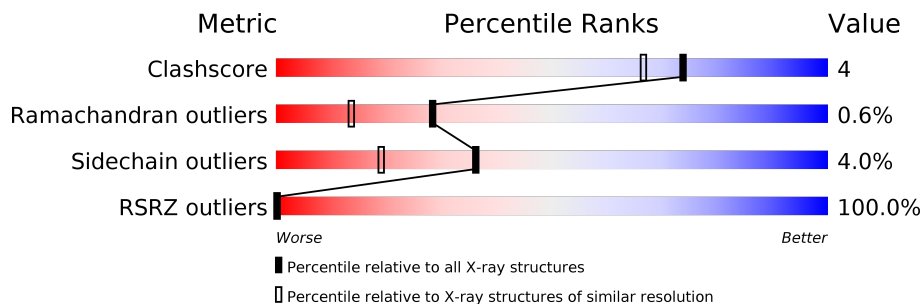
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (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 ≥ 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>89%</div> <div>9%</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 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.

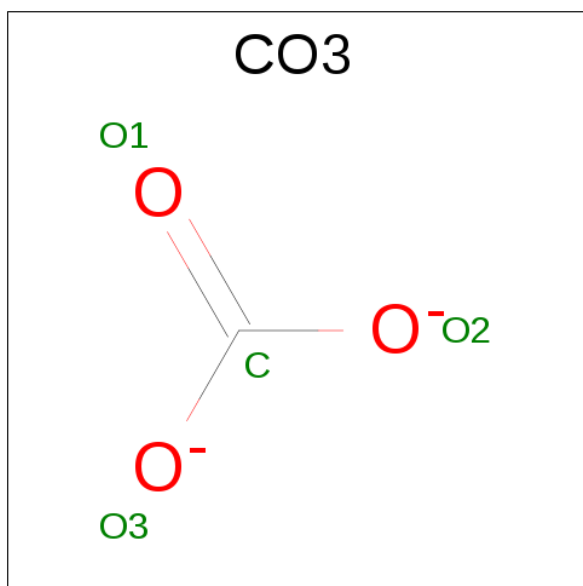
- Molecule 1 is a protein called SERUM TRANSFERRIN.

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	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

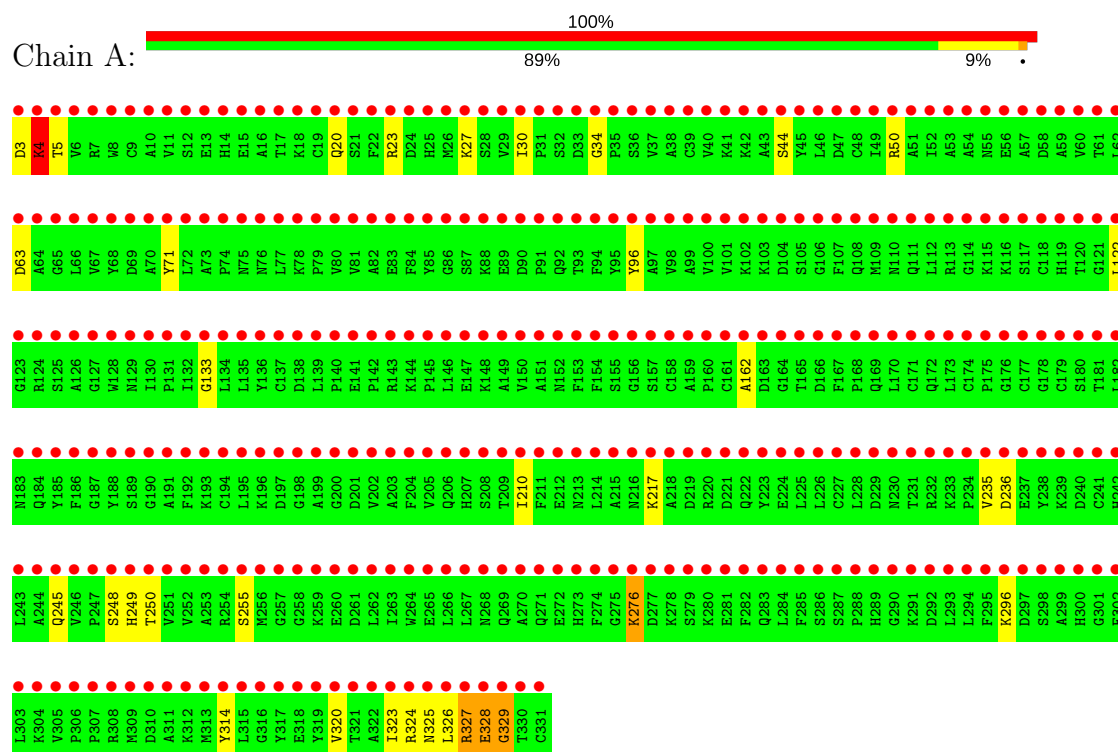
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total 139	O 139	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: 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)	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 ²)	23.1	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

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.*

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: 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 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	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%)	28 13

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%)	36	19

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 [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.

No monomer is involved in short contacts.

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, 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%)	8.47	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	25.1
1	A	211	PHE	22.9
1	A	68	TYR	22.4
1	A	106	GLY	21.4
1	A	247	PRO	20.6
1	A	329	GLY	20.5
1	A	3	ASP	19.8
1	A	29	VAL	18.5
1	A	229	ASP	18.1
1	A	33	ASP	18.0
1	A	205	VAL	17.1
1	A	330	THR	17.0
1	A	274	PHE	16.8
1	A	30	ILE	16.5
1	A	317	TYR	16.4
1	A	331	CYS	16.3
1	A	222	GLN	16.1
1	A	328	GLU	15.7
1	A	191	ALA	14.7
1	A	154	PHE	14.7
1	A	255	SER	14.4
1	A	128	TRP	14.3
1	A	248	SER	13.7
1	A	326	LEU	13.6
1	A	87	SER	13.6
1	A	231	THR	13.4
1	A	61	THR	13.4

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Mol	Chain	Res	Type	RSRZ
1	A	50	ARG	13.3
1	A	264	TRP	13.3
1	A	100	VAL	13.2
1	A	178	GLY	13.1
1	A	153	PHE	13.0
1	A	204	PHE	13.0
1	A	258	GLY	13.0
1	A	244	ALA	12.8
1	A	71	TYR	12.7
1	A	168	PRO	12.7
1	A	113	ARG	12.6
1	A	305	VAL	12.4
1	A	325	ASN	12.3
1	A	210	ILE	12.3
1	A	186	PHE	12.3
1	A	109	MET	12.2
1	A	51	ALA	12.1
1	A	104	ASP	12.1
1	A	165	THR	12.1
1	A	163	ASP	12.1
1	A	35	PRO	12.1
1	A	324	ARG	12.0
1	A	58	ASP	12.0
1	A	209	THR	11.9
1	A	316	GLY	11.7
1	A	189	SER	11.7
1	A	277	ASP	11.7
1	A	228	LEU	11.7
1	A	236	ASP	11.7
1	A	32	SER	11.6
1	A	117	SER	11.6
1	A	302	PHE	11.6
1	A	288	PRO	11.6
1	A	52	ILE	11.6
1	A	73	ALA	11.6
1	A	196	LYS	11.5
1	A	280	LYS	11.5
1	A	81	VAL	11.4
1	A	181	THR	11.3
1	A	69	ASP	11.1
1	A	134	LEU	11.1
1	A	308	ARG	11.1

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Mol	Chain	Res	Type	RSRZ
1	A	300	HIS	11.1
1	A	246	VAL	11.0
1	A	259	LYS	11.0
1	A	144	LYS	10.9
1	A	96	TYR	10.9
1	A	65	GLY	10.9
1	A	314	TYR	10.9
1	A	5	THR	10.7
1	A	215	ALA	10.7
1	A	17	THR	10.7
1	A	19	CYS	10.7
1	A	170	LEU	10.7
1	A	38	ALA	10.6
1	A	43	ALA	10.5
1	A	150	VAL	10.5
1	A	95	TYR	10.3
1	A	152	ASN	10.3
1	A	114	GLY	10.3
1	A	230	ASN	10.3
1	A	77	LEU	10.3
1	A	151	ALA	10.2
1	A	49	ILE	10.2
1	A	110	ASN	9.9
1	A	156	GLY	9.9
1	A	239	LYS	9.8
1	A	263	ILE	9.8
1	A	173	LEU	9.8
1	A	6	VAL	9.8
1	A	221	ASP	9.8
1	A	282	PHE	9.7
1	A	64	ALA	9.7
1	A	127	GLY	9.6
1	A	31	PRO	9.6
1	A	135	LEU	9.6
1	A	157	SER	9.5
1	A	194	CYS	9.5
1	A	321	THR	9.4
1	A	67	VAL	9.4
1	A	192	PHE	9.3
1	A	293	LEU	9.3
1	A	22	PHE	9.3
1	A	20	GLN	9.2

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Mol	Chain	Res	Type	RSRZ
1	A	262	LEU	9.2
1	A	136	TYR	9.1
1	A	250	THR	8.9
1	A	237	GLU	8.9
1	A	90	ASP	8.8
1	A	123	GLY	8.8
1	A	285	PHE	8.8
1	A	232	ARG	8.8
1	A	202	VAL	8.7
1	A	139	LEU	8.7
1	A	34	GLY	8.7
1	A	24	ASP	8.7
1	A	234	PRO	8.7
1	A	75	ASN	8.7
1	A	88	LYS	8.7
1	A	146	LEU	8.6
1	A	241	CYS	8.6
1	A	12	SER	8.5
1	A	132	ILE	8.5
1	A	147	GLU	8.5
1	A	319	TYR	8.4
1	A	98	VAL	8.4
1	A	82	ALA	8.4
1	A	80	VAL	8.4
1	A	27	LYS	8.4
1	A	74	PRO	8.4
1	A	76	ASN	8.4
1	A	140	PRO	8.3
1	A	323	ILE	8.3
1	A	45	TYR	8.3
1	A	235	VAL	8.2
1	A	273	HIS	8.2
1	A	130	ILE	8.2
1	A	266	LEU	8.1
1	A	251	VAL	8.1
1	A	93	THR	8.0
1	A	301	GLY	8.0
1	A	62	LEU	8.0
1	A	101	VAL	8.0
1	A	118	CYS	8.0
1	A	214	LEU	8.0
1	A	217	LYS	7.9

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Mol	Chain	Res	Type	RSRZ
1	A	142	PRO	7.9
1	A	120	THR	7.9
1	A	182	LEU	7.9
1	A	137	CYS	7.9
1	A	195	LEU	7.8
1	A	84	PHE	7.8
1	A	261	ASP	7.8
1	A	129	ASN	7.8
1	A	103	LYS	7.8
1	A	240	ASP	7.8
1	A	238	TYR	7.7
1	A	199	ALA	7.7
1	A	53	ALA	7.6
1	A	177	CYS	7.6
1	A	131	PRO	7.6
1	A	14	HIS	7.5
1	A	160	PRO	7.5
1	A	322	ALA	7.5
1	A	39	CYS	7.5
1	A	169	GLN	7.5
1	A	125	SER	7.5
1	A	8	TRP	7.5
1	A	46	LEU	7.4
1	A	107	PHE	7.4
1	A	203	ALA	7.4
1	A	208	SER	7.4
1	A	176	GLY	7.4
1	A	249	HIS	7.4
1	A	13	GLU	7.3
1	A	48	CYS	7.3
1	A	253	ALA	7.3
1	A	206	GLN	7.3
1	A	162	ALA	7.3
1	A	66	LEU	7.3
1	A	179	CYS	7.3
1	A	89	GLU	7.2
1	A	28	SER	7.2
1	A	94	PHE	7.2
1	A	25	HIS	7.2
1	A	166	ASP	7.2
1	A	97	ALA	7.1
1	A	126	ALA	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	312	LYS	7.1
1	A	105	SER	7.0
1	A	315	LEU	7.0
1	A	36	SER	6.9
1	A	295	PHE	6.9
1	A	37	VAL	6.9
1	A	63	ASP	6.9
1	A	158	CYS	6.9
1	A	299	ALA	6.9
1	A	213	ASN	6.8
1	A	78	LYS	6.8
1	A	175	PRO	6.7
1	A	7	ARG	6.7
1	A	243	LEU	6.6
1	A	291	LYS	6.6
1	A	185	TYR	6.6
1	A	164	GLY	6.6
1	A	310	ASP	6.6
1	A	278	LYS	6.6
1	A	161	CYS	6.6
1	A	309	MET	6.5
1	A	284	LEU	6.5
1	A	143	ARG	6.5
1	A	91	PRO	6.5
1	A	183	ASN	6.5
1	A	265	GLU	6.5
1	A	41	LYS	6.5
1	A	72	LEU	6.5
1	A	171	CYS	6.4
1	A	294	LEU	6.4
1	A	289	HIS	6.4
1	A	188	TYR	6.4
1	A	11	VAL	6.4
1	A	256	MET	6.3
1	A	56	GLU	6.3
1	A	304	LYS	6.3
1	A	4	LYS	6.2
1	A	272	GLU	6.2
1	A	303	LEU	6.1
1	A	218	ALA	6.1
1	A	269	GLN	6.1
1	A	112	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	306	PRO	6.0
1	A	21	SER	6.0
1	A	60	VAL	6.0
1	A	148	LYS	6.0
1	A	227	CYS	5.9
1	A	223	TYR	5.9
1	A	116	LYS	5.9
1	A	245	GLN	5.9
1	A	155	SER	5.9
1	A	320	VAL	5.8
1	A	200	GLY	5.8
1	A	268	ASN	5.8
1	A	57	ALA	5.8
1	A	260	GLU	5.8
1	A	190	GLY	5.8
1	A	271	GLN	5.8
1	A	198	GLY	5.7
1	A	16	ALA	5.7
1	A	193	LYS	5.7
1	A	138	ASP	5.7
1	A	141	GLU	5.7
1	A	283	GLN	5.6
1	A	59	ALA	5.6
1	A	23	ARG	5.6
1	A	257	GLY	5.6
1	A	85	TYR	5.5
1	A	327	ARG	5.5
1	A	318	GLU	5.4
1	A	197	ASP	5.4
1	A	281	GLU	5.4
1	A	313	MET	5.4
1	A	145	PRO	5.4
1	A	174	CYS	5.4
1	A	270	ALA	5.4
1	A	92	GLN	5.4
1	A	225	LEU	5.3
1	A	267	LEU	5.3
1	A	115	LYS	5.3
1	A	86	GLY	5.2
1	A	9	CYS	5.2
1	A	252	VAL	5.2
1	A	286	SER	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	290	GLY	5.1
1	A	124	ARG	5.1
1	A	201	ASP	5.0
1	A	226	LEU	5.0
1	A	40	VAL	5.0
1	A	26	MET	4.9
1	A	159	ALA	4.9
1	A	292	ASP	4.8
1	A	70	ALA	4.8
1	A	54	ALA	4.8
1	A	122	LEU	4.8
1	A	276	LYS	4.8
1	A	10	ALA	4.8
1	A	311	ALA	4.8
1	A	42	LYS	4.7
1	A	99	ALA	4.6
1	A	111	GLN	4.6
1	A	187	GLY	4.6
1	A	275	GLY	4.4
1	A	172	GLN	4.4
1	A	184	GLN	4.4
1	A	216	ASN	4.4
1	A	119	HIS	4.3
1	A	242	HIS	4.3
1	A	254	ARG	4.2
1	A	220	ARG	4.2
1	A	83	GLU	4.1
1	A	287	SER	4.1
1	A	149	ALA	4.1
1	A	219	ASP	4.1
1	A	224	GLU	4.1
1	A	102	LYS	4.1
1	A	44	SER	4.1
1	A	233	LYS	3.9
1	A	180	SER	3.9
1	A	297	ASP	3.8
1	A	296	LYS	3.8
1	A	47	ASP	3.7
1	A	133	GLY	3.7
1	A	212	GLU	3.5
1	A	121	GLY	3.4
1	A	108	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	79	PRO	3.2
1	A	15	GLU	3.1
1	A	55	ASN	3.1
1	A	207	HIS	3.0
1	A	279	SER	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 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(Å ²)	Q<0.9
2	CO3	A	338	4/4	0.19	0.95	6.32	15,17,17,18	0
3	FE	A	339	1/1	0.73	0.50	0.35	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.