Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 12:41 PM EDT

PDB ID	:	1D4N
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	:	1999-10-04
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

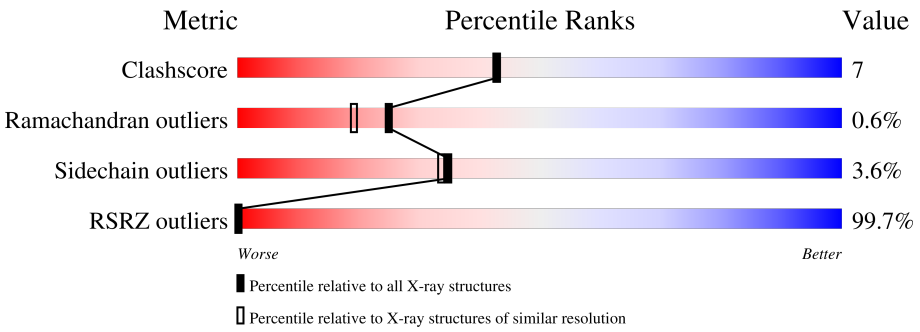
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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 <=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	100% 83% 16% •

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.

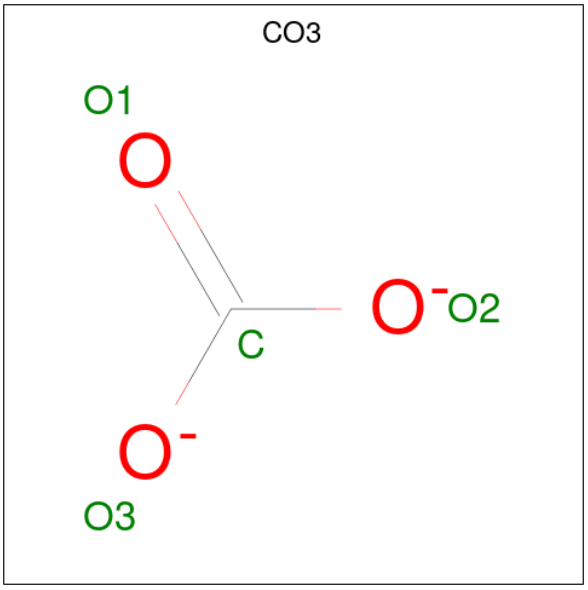
- Molecule 1 is a protein called TRANSFERRIN.

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 mutation	UNP P02787

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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
			Total	Fe		
3	A	1	1	1	0	0

- Molecule 4 is water.

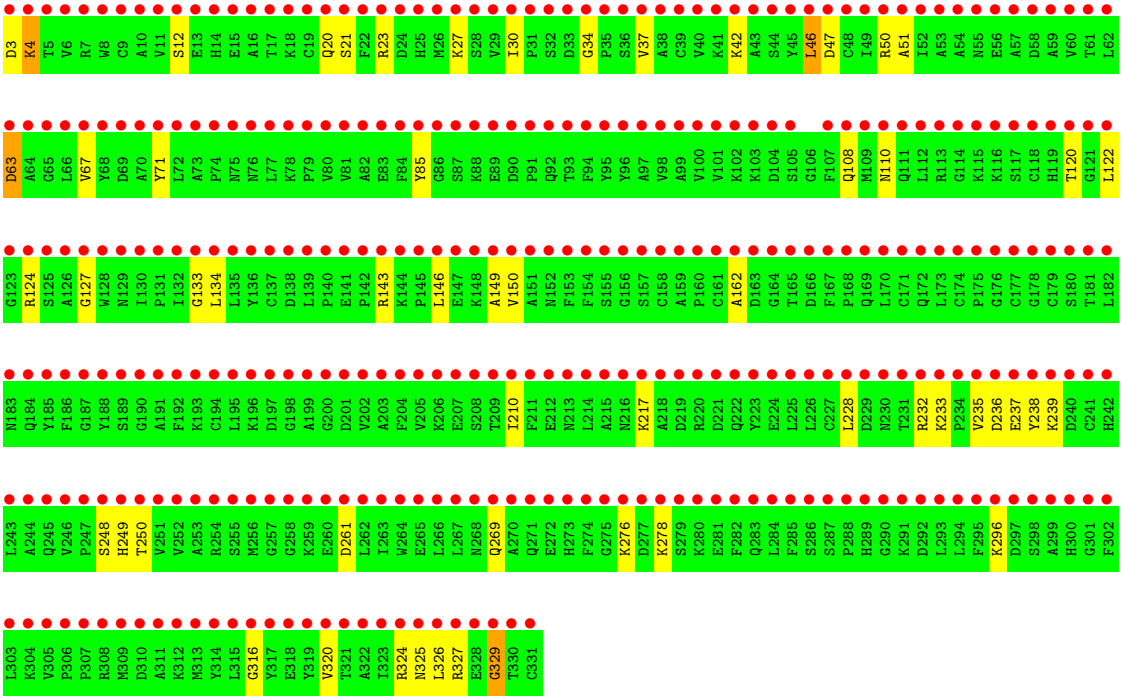
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	135	135	135	0	0

3 Residue-property plots (i)

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: TRANSFERRIN

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	0.59 (at 2.00Å)	Xtriage
Refinement program	XTALVIEW, X-PLOR 3.851	Depositor
R, R_{free}	0.179 , 0.218 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
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
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	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^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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.46	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:46:LEU:O	1:A:50:ARG:HG2	2.06	0.55
1:A:124:ARG:NH2	2:A:338:CO3:O2	2.40	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:42:LYS:HD2	1:A:47:ASP:HB3	2.00	0.44
1:A:108:GLN:NE2	1:A:108:GLN:HA	2.32	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:HB3	1:A:278:LYS:HE2	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 (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%)	307 (94%)	18 (6%)	2 (1%)	25 19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
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%)	264 (96%)	10 (4%)	35 34

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

Sometimes 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 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.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	11.97	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	48.3
1	A	284	LEU	44.9
1	A	192	PHE	37.2
1	A	282	PHE	36.3
1	A	200	GLY	36.3
1	A	229	ASP	35.9
1	A	209	THR	34.5
1	A	182	LEU	33.8
1	A	330	THR	33.6
1	A	228	LEU	32.3
1	A	205	VAL	31.6
1	A	171	CYS	30.2
1	A	303	LEU	30.0
1	A	135	LEU	29.4
1	A	178	GLY	28.8
1	A	75	ASN	28.5
1	A	73	ALA	28.1
1	A	137	CYS	27.9
1	A	117	SER	26.8
1	A	213	ASN	26.7
1	A	309	MET	26.3
1	A	210	ILE	26.2
1	A	283	GLN	26.2
1	A	288	PRO	26.0
1	A	40	VAL	25.4
1	A	166	ASP	25.2
1	A	199	ALA	24.9

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Mol	Chain	Res	Type	RSRZ
1	A	194	CYS	24.8
1	A	43	ALA	24.1
1	A	90	ASP	23.8
1	A	91	PRO	23.2
1	A	128	TRP	23.0
1	A	275	GLY	22.7
1	A	227	CYS	22.6
1	A	98	VAL	22.4
1	A	263	ILE	22.3
1	A	211	PHE	21.8
1	A	89	GLU	21.8
1	A	308	ARG	21.5
1	A	84	PHE	21.2
1	A	87	SER	20.5
1	A	52	ILE	20.5
1	A	233	LYS	20.4
1	A	305	VAL	20.3
1	A	304	LYS	20.2
1	A	237	GLU	20.0
1	A	195	LEU	19.8
1	A	138	ASP	19.7
1	A	203	ALA	19.7
1	A	202	VAL	19.4
1	A	236	ASP	19.3
1	A	22	PHE	19.2
1	A	136	TYR	19.1
1	A	163	ASP	18.6
1	A	134	LEU	18.3
1	A	240	ASP	18.0
1	A	81	VAL	18.0
1	A	31	PRO	18.0
1	A	177	CYS	17.9
1	A	300	HIS	17.9
1	A	34	GLY	17.9
1	A	35	PRO	17.5
1	A	239	LYS	17.5
1	A	131	PRO	17.4
1	A	242	HIS	17.3
1	A	165	THR	17.3
1	A	38	ALA	17.2
1	A	234	PRO	17.0
1	A	259	LYS	17.0

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Mol	Chain	Res	Type	RSRZ
1	A	5	THR	16.8
1	A	201	ASP	16.8
1	A	310	ASP	16.7
1	A	42	LYS	16.6
1	A	329	GLY	16.3
1	A	231	THR	16.3
1	A	197	ASP	16.0
1	A	196	LYS	15.9
1	A	51	ALA	15.8
1	A	68	TYR	15.7
1	A	16	ALA	15.6
1	A	173	LEU	15.5
1	A	243	LEU	15.5
1	A	331	CYS	15.3
1	A	274	PHE	15.2
1	A	198	GLY	15.2
1	A	61	THR	15.1
1	A	72	LEU	15.1
1	A	3	ASP	15.0
1	A	7	ARG	15.0
1	A	6	VAL	14.8
1	A	287	SER	14.4
1	A	71	TYR	14.4
1	A	37	VAL	14.4
1	A	206	LYS	14.3
1	A	193	LYS	14.3
1	A	76	ASN	14.3
1	A	172	GLN	14.2
1	A	156	GLY	14.1
1	A	255	SER	14.0
1	A	183	ASN	14.0
1	A	324	ARG	13.9
1	A	46	LEU	13.9
1	A	32	SER	13.9
1	A	56	GLU	13.8
1	A	328	GLU	13.7
1	A	295	PHE	13.7
1	A	170	LEU	13.6
1	A	113	ARG	13.5
1	A	168	PRO	13.5
1	A	169	GLN	13.5
1	A	244	ALA	13.3

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Mol	Chain	Res	Type	RSRZ
1	A	289	HIS	13.3
1	A	176	GLY	13.2
1	A	175	PRO	13.2
1	A	77	LEU	13.1
1	A	47	ASP	13.0
1	A	285	PHE	12.9
1	A	25	HIS	12.9
1	A	24	ASP	12.6
1	A	238	TYR	12.5
1	A	280	LYS	12.5
1	A	88	LYS	12.5
1	A	312	LYS	12.3
1	A	96	TYR	12.2
1	A	179	CYS	12.2
1	A	39	CYS	12.2
1	A	8	TRP	12.1
1	A	294	LEU	12.0
1	A	181	THR	12.0
1	A	141	GLU	11.9
1	A	55	ASN	11.9
1	A	326	LEU	11.9
1	A	157	SER	11.7
1	A	276	LYS	11.6
1	A	154	PHE	11.5
1	A	261	ASP	11.4
1	A	127	GLY	11.4
1	A	317	TYR	11.4
1	A	41	LYS	11.2
1	A	129	ASN	11.1
1	A	82	ALA	11.0
1	A	185	TYR	10.9
1	A	100	VAL	10.9
1	A	74	PRO	10.8
1	A	313	MET	10.8
1	A	204	PHE	10.7
1	A	125	SER	10.7
1	A	118	CYS	10.6
1	A	191	ALA	10.6
1	A	235	VAL	10.6
1	A	28	SER	10.5
1	A	112	LEU	10.5
1	A	30	ILE	10.4

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Mol	Chain	Res	Type	RSRZ
1	A	264	TRP	10.4
1	A	167	PHE	10.3
1	A	94	PHE	10.3
1	A	17	THR	10.3
1	A	33	ASP	10.3
1	A	215	ALA	10.2
1	A	132	ILE	10.2
1	A	222	GLN	10.2
1	A	277	ASP	10.2
1	A	257	GLY	10.1
1	A	164	GLY	10.0
1	A	80	VAL	9.9
1	A	241	CYS	9.9
1	A	258	GLY	9.8
1	A	219	ASP	9.8
1	A	50	ARG	9.7
1	A	225	LEU	9.6
1	A	19	CYS	9.6
1	A	12	SER	9.5
1	A	189	SER	9.4
1	A	271	GLN	9.3
1	A	101	VAL	9.3
1	A	116	LYS	9.2
1	A	14	HIS	9.2
1	A	67	VAL	9.2
1	A	103	LYS	9.0
1	A	48	CYS	9.0
1	A	85	TYR	8.9
1	A	208	SER	8.9
1	A	13	GLU	8.7
1	A	226	LEU	8.6
1	A	9	CYS	8.6
1	A	62	LEU	8.5
1	A	249	HIS	8.5
1	A	93	THR	8.4
1	A	256	MET	8.4
1	A	159	ALA	8.4
1	A	58	ASP	8.3
1	A	147	GLU	8.3
1	A	325	ASN	8.2
1	A	151	ALA	8.2
1	A	299	ALA	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	63	ASP	8.2
1	A	92	GLN	8.1
1	A	115	LYS	8.1
1	A	36	SER	8.1
1	A	216	ASN	8.1
1	A	174	CYS	8.1
1	A	190	GLY	8.0
1	A	26	MET	8.0
1	A	150	VAL	7.9
1	A	323	ILE	7.8
1	A	281	GLU	7.8
1	A	110	ASN	7.7
1	A	49	ILE	7.7
1	A	214	LEU	7.6
1	A	139	LEU	7.6
1	A	262	LEU	7.5
1	A	23	ARG	7.4
1	A	15	GLU	7.4
1	A	267	LEU	7.3
1	A	83	GLU	7.3
1	A	64	ALA	7.3
1	A	278	LYS	7.2
1	A	302	PHE	7.2
1	A	265	GLU	7.1
1	A	153	PHE	7.1
1	A	109	MET	7.0
1	A	306	PRO	7.0
1	A	133	GLY	7.0
1	A	95	TYR	7.0
1	A	293	LEU	6.9
1	A	320	VAL	6.9
1	A	322	ALA	6.8
1	A	4	LYS	6.8
1	A	70	ALA	6.8
1	A	86	GLY	6.8
1	A	161	CYS	6.7
1	A	152	ASN	6.7
1	A	188	TYR	6.7
1	A	11	VAL	6.7
1	A	260	GLU	6.6
1	A	124	ARG	6.6
1	A	114	GLY	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	223	TYR	6.5
1	A	291	LYS	6.5
1	A	143	ARG	6.5
1	A	301	GLY	6.5
1	A	105	SER	6.4
1	A	246	VAL	6.4
1	A	54	ALA	6.4
1	A	20	GLN	6.3
1	A	232	ARG	6.3
1	A	53	ALA	6.3
1	A	78	LYS	6.3
1	A	102	LYS	6.3
1	A	266	LEU	6.2
1	A	311	ALA	6.2
1	A	207	GLU	6.1
1	A	247	PRO	6.1
1	A	218	ALA	6.0
1	A	126	ALA	6.0
1	A	318	GLU	5.9
1	A	120	THR	5.9
1	A	314	TYR	5.9
1	A	212	GLU	5.9
1	A	123	GLY	5.8
1	A	186	PHE	5.8
1	A	59	ALA	5.7
1	A	27	LYS	5.7
1	A	319	TYR	5.7
1	A	254	ARG	5.7
1	A	130	ILE	5.6
1	A	45	TYR	5.6
1	A	316	GLY	5.5
1	A	149	ALA	5.5
1	A	298	SER	5.5
1	A	327	ARG	5.4
1	A	286	SER	5.4
1	A	184	GLN	5.4
1	A	57	ALA	5.4
1	A	251	VAL	5.3
1	A	315	LEU	5.3
1	A	119	HIS	5.2
1	A	252	VAL	5.2
1	A	65	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	307	PRO	5.2
1	A	111	GLN	5.1
1	A	146	LEU	5.0
1	A	250	THR	5.0
1	A	107	PHE	5.0
1	A	21	SER	4.9
1	A	279	SER	4.9
1	A	66	LEU	4.8
1	A	122	LEU	4.8
1	A	10	ALA	4.7
1	A	248	SER	4.7
1	A	321	THR	4.6
1	A	104	ASP	4.6
1	A	44	SER	4.6
1	A	292	ASP	4.5
1	A	69	ASP	4.5
1	A	162	ALA	4.5
1	A	158	CYS	4.5
1	A	121	GLY	4.4
1	A	224	GLU	4.4
1	A	155	SER	4.4
1	A	140	PRO	4.3
1	A	142	PRO	4.3
1	A	290	GLY	4.3
1	A	296	LYS	4.3
1	A	29	VAL	4.3
1	A	60	VAL	4.2
1	A	245	GLN	4.2
1	A	79	PRO	4.2
1	A	97	ALA	4.2
1	A	99	ALA	4.1
1	A	253	ALA	3.9
1	A	18	LYS	3.9
1	A	145	PRO	3.8
1	A	160	PRO	3.8
1	A	108	GLN	3.7
1	A	148	LYS	3.7
1	A	180	SER	3.4
1	A	144	LYS	3.3
1	A	297	ASP	3.2
1	A	220	ARG	3.1
1	A	273	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	270	ALA	3.1
1	A	187	GLY	3.1
1	A	269	GLN	2.9
1	A	221	ASP	2.6
1	A	268	ASN	2.5
1	A	272	GLU	2.4
1	A	217	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
3	FE	A	339	1/1	-0.41	0.44	16,16,16,16	0
2	CO3	A	338	4/4	-0.24	0.54	11,13,16,17	0

6.5 Other polymers (i)

There are no such residues in this entry.