W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 22, 2024 – 04:56 AM EDT

PDB ID	:	3S9L
Title	:	Complex between transferrin receptor 1 and transferrin with iron in the N-Lobe, cryocooled 2
Authors	:	Eckenroth, B.E.; Steere, A.N.; Mason, A.B.; Everse, S.J.
Deposited on	:	2011-06-01
Resolution	:	3.22 Å(reported)

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

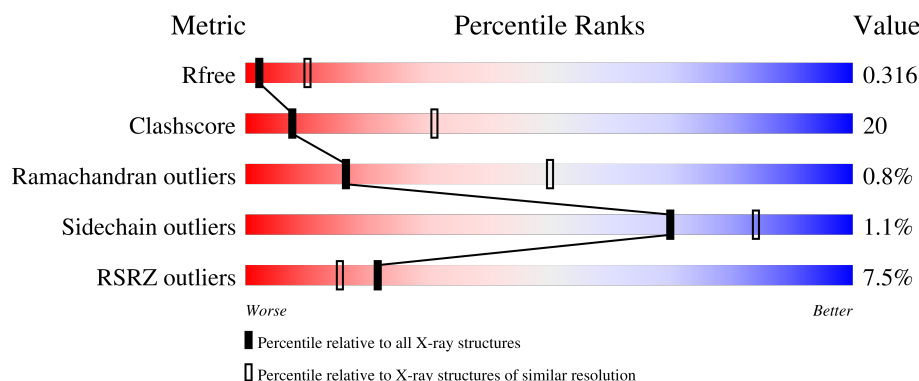|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.22 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	Percentile Ranks	Value
Rfree		0.316
Clashscore		20
Ramachandran outliers		0.8%
Sidechain outliers		1.1%
RSRZ outliers		7.5%

Worse *Better*

▌ Percentile relative to all X-ray structures

▐ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1638 (3.24-3.20)
Clashscore	180529	1778 (3.24-3.20)
Ramachandran outliers	177936	1751 (3.24-3.20)
Sidechain outliers	177891	1750 (3.24-3.20)
RSRZ outliers	164620	1639 (3.24-3.20)

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	654	3% / 59% / 37% / ••
1	B	654	10% / 65% / 32% / ••
2	C	693	8% / 55% / 19% / • / 26%
2	D	693	5% / 55% / 15% / 30%

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
6	CO3	D	905	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 16713 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 receptor protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			4949	3169	828	938	14			
1	B	639	Total	C	N	O	S	0	0	0
			4800	3064	799	923	14			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	VAL	-	expression tag	UNP P02786
A	108	PRO	-	expression tag	UNP P02786
A	109	ASP	-	expression tag	UNP P02786
A	110	LYS	-	expression tag	UNP P02786
A	111	HIS	-	expression tag	UNP P02786
A	112	HIS	-	expression tag	UNP P02786
A	113	HIS	-	expression tag	UNP P02786
A	114	HIS	-	expression tag	UNP P02786
A	115	HIS	-	expression tag	UNP P02786
A	116	HIS	-	expression tag	UNP P02786
A	117	ILE	-	expression tag	UNP P02786
A	118	GLU	-	expression tag	UNP P02786
A	119	GLY	-	expression tag	UNP P02786
A	142	SER	GLY	SEE REMARK 999	UNP P02786
B	107	VAL	-	expression tag	UNP P02786
B	108	PRO	-	expression tag	UNP P02786
B	109	ASP	-	expression tag	UNP P02786
B	110	LYS	-	expression tag	UNP P02786
B	111	HIS	-	expression tag	UNP P02786
B	112	HIS	-	expression tag	UNP P02786
B	113	HIS	-	expression tag	UNP P02786
B	114	HIS	-	expression tag	UNP P02786
B	115	HIS	-	expression tag	UNP P02786
B	116	HIS	-	expression tag	UNP P02786
B	117	ILE	-	expression tag	UNP P02786

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Chain	Residue	Modelled	Actual	Comment	Reference
B	118	GLU	-	expression tag	UNP P02786
B	119	GLY	-	expression tag	UNP P02786
B	142	SER	GLY	SEE REMARK 999	UNP P02786

- Molecule 2 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	515	Total 3650	C 2275	N 615	O 725	S 35	0	0	0
2	D	487	Total 3274	C 1997	N 569	O 675	S 33	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	VAL	-	expression tag	UNP P02787
C	-12	PRO	-	expression tag	UNP P02787
C	-11	ASP	-	expression tag	UNP P02787
C	-10	LYS	-	expression tag	UNP P02787
C	-9	HIS	-	expression tag	UNP P02787
C	-8	HIS	-	expression tag	UNP P02787
C	-7	HIS	-	expression tag	UNP P02787
C	-6	HIS	-	expression tag	UNP P02787
C	-5	HIS	-	expression tag	UNP P02787
C	-4	HIS	-	expression tag	UNP P02787
C	-3	ILE	-	expression tag	UNP P02787
C	-2	GLU	-	expression tag	UNP P02787
C	-1	GLY	-	expression tag	UNP P02787
C	0	ARG	-	expression tag	UNP P02787
C	413	ASP	ASN	engineered mutation	UNP P02787
C	426	PHE	TYR	engineered mutation	UNP P02787
C	429	VAL	ILE	SEE REMARK 999	UNP P02787
C	517	PHE	TYR	engineered mutation	UNP P02787
C	611	ASP	ASN	engineered mutation	UNP P02787
D	-13	VAL	-	expression tag	UNP P02787
D	-12	PRO	-	expression tag	UNP P02787
D	-11	ASP	-	expression tag	UNP P02787
D	-10	LYS	-	expression tag	UNP P02787
D	-9	HIS	-	expression tag	UNP P02787
D	-8	HIS	-	expression tag	UNP P02787
D	-7	HIS	-	expression tag	UNP P02787
D	-6	HIS	-	expression tag	UNP P02787

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP P02787
D	-4	HIS	-	expression tag	UNP P02787
D	-3	ILE	-	expression tag	UNP P02787
D	-2	GLU	-	expression tag	UNP P02787
D	-1	GLY	-	expression tag	UNP P02787
D	0	ARG	-	expression tag	UNP P02787
D	413	ASP	ASN	engineered mutation	UNP P02787
D	426	PHE	TYR	engineered mutation	UNP P02787
D	429	VAL	ILE	SEE REMARK 999	UNP P02787
D	517	PHE	TYR	engineered mutation	UNP P02787
D	611	ASP	ASN	engineered mutation	UNP P02787

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
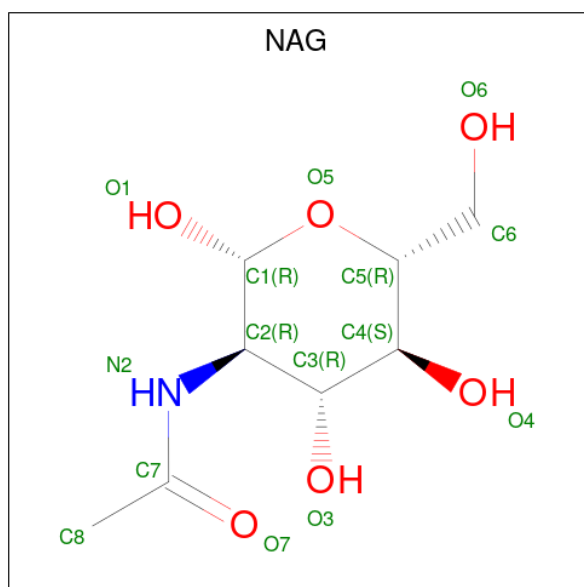
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total Ca 1 1		0	0

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total Fe 1 1		0	0
5	D	1	Total Fe 1 1		0	0

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).
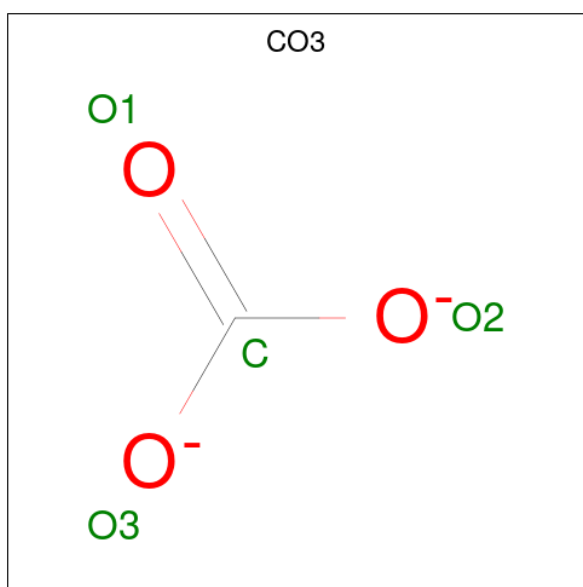
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total C O 4 1 3			0	0
6	D	1	Total C O 4 1 3			0	0

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: Transferrin receptor protein 1

Chain A:

• Molecule 1: Transferrin receptor protein 1

Chain B:

• Molecule 2: Serotransferrin

Chain C:

• Molecule 2: Serotransferrin

Chain D:
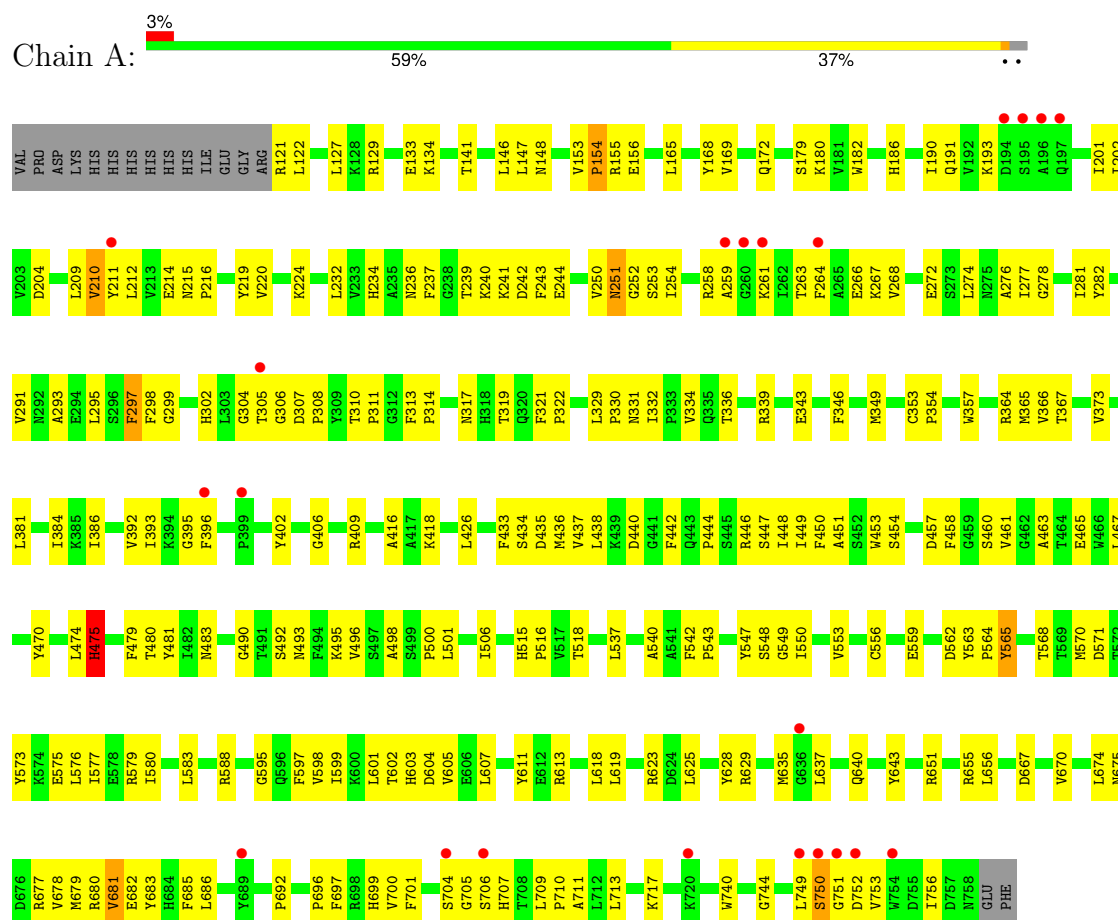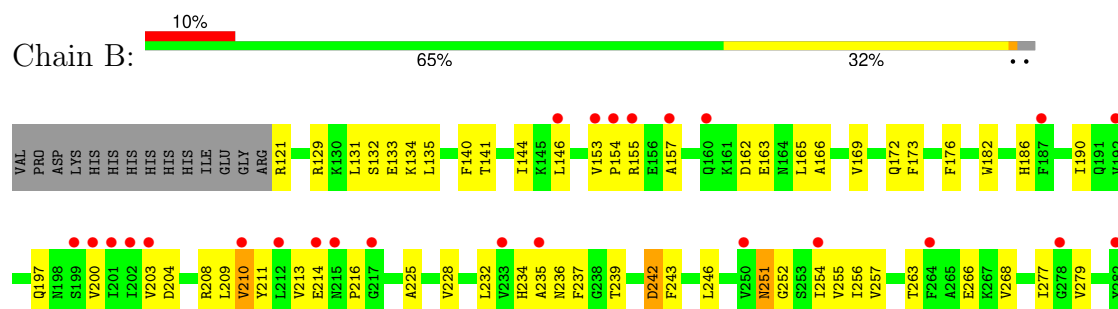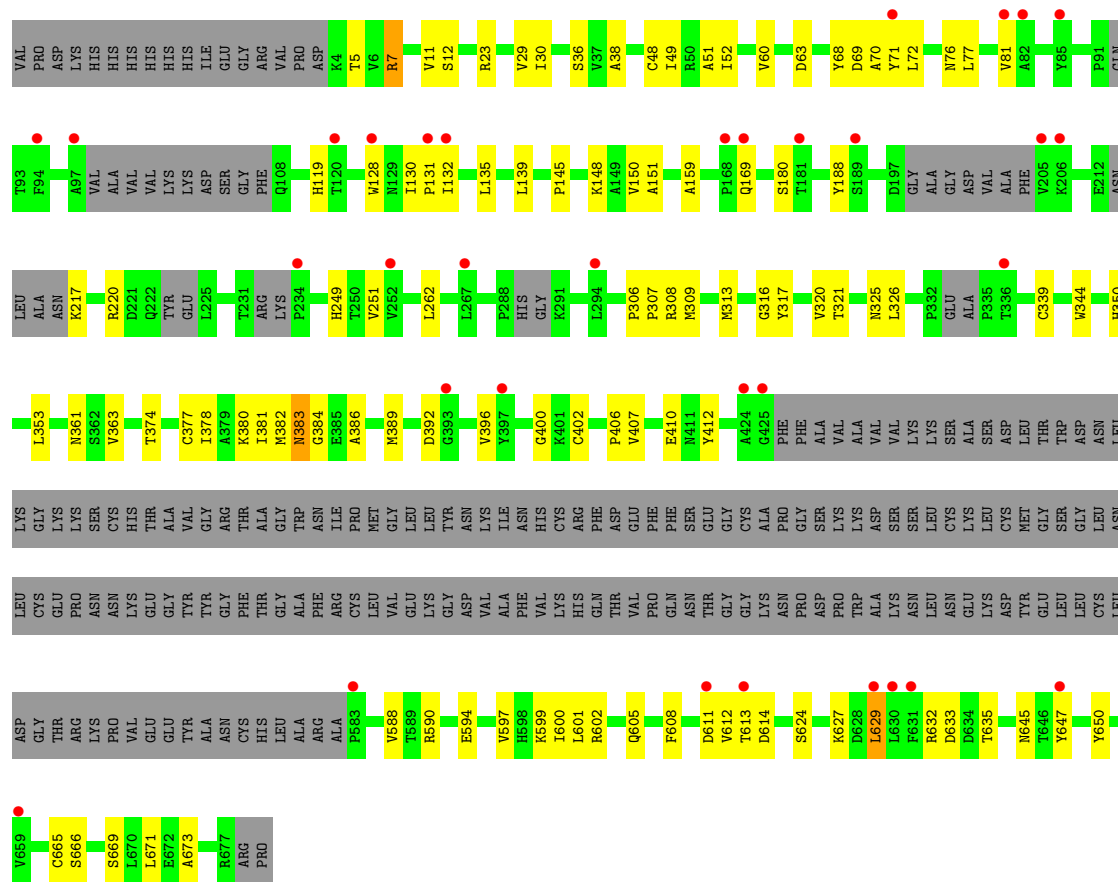
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	231.68Å 231.68Å 168.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.22 30.00 – 3.22	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.22) 99.3 (30.00-3.22)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 3.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.271 , 0.314 0.273 , 0.316	Depositor DCC
R_{free} test set	7464 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å^2)	89.1	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 88.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16713	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FE, CA, 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	0.42	0/5068	0.60	0/6897
1	B	0.42	0/4916	0.57	1/6718 (0.0%)
2	C	0.34	0/3725	0.52	0/5095
2	D	0.29	0/3327	0.49	0/4546
All	All	0.38	0/17036	0.55	1/23256 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	579	ARG	NE-CZ-NH2	-5.21	117.70	120.30

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	4949	0	4754	242	0
1	B	4800	0	4434	184	0
2	C	3650	0	3184	121	0
2	D	3274	0	2660	85	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0

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PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	C	4	0	0	0	0
6	D	4	0	0	3	0
All	All	16713	0	15058	625	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 20.

The worst 5 of 625 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:B:489:LEU:HD12	1:B:558:CYS:SG	1.56	1.43
1:B:412:TRP:CZ3	1:B:569:THR:HG23	1.52	1.42
1:B:412:TRP:CZ3	1:B:569:THR:CG2	2.21	1.22
2:C:58:ASP:CG	2:C:259:LYS:HZ1	1.49	1.14
1:A:677:ARG:NH1	1:A:751:GLY:HA2	1.63	1.12

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	636/654 (97%)	588 (92%)	43 (7%)	5 (1%)	16	50
1	B	637/654 (97%)	603 (95%)	32 (5%)	2 (0%)	37	68
2	C	509/693 (73%)	464 (91%)	39 (8%)	6 (1%)	11	42
2	D	467/693 (67%)	434 (93%)	29 (6%)	4 (1%)	14	48
All	All	2249/2694 (84%)	2089 (93%)	143 (6%)	17 (1%)	16	50

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	VAL
1	A	681	VAL
2	C	125	SER
2	D	613	THR
2	D	629	LEU

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	521/562 (93%)	515 (99%)	6 (1%)	67	83
1	B	483/562 (86%)	477 (99%)	6 (1%)	67	83
2	C	353/585 (60%)	349 (99%)	4 (1%)	70	84
2	D	291/585 (50%)	289 (99%)	2 (1%)	81	90
All	All	1648/2294 (72%)	1630 (99%)	18 (1%)	70	84

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	241	CYS
2	D	383	ASN
2	D	7	ARG
1	B	251	ASN
2	C	129	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	584	ASN
2	D	585	HIS
2	C	585	HIS
2	D	325	ASN
2	D	604	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#|Z| > 2$
3	NAG	B	903	1	14,14,15	0.44	0	17,19,21	1.16	2 (11%)
3	NAG	A	903	1	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
6	CO3	C	905	5	3,3,3	0.29	0	2,3,3	0.26	0
6	CO3	D	905	5	3,3,3	0.23	0	2,3,3	0.13	0

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
3	NAG	B	903	1	-	0/6/23/26	0/1/1/1
3	NAG	A	903	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	903	NAG	C8-C7-N2	2.31	119.94	116.12
3	A	903	NAG	C8-C7-N2	2.30	119.94	116.12
3	B	903	NAG	C2-N2-C7	-2.18	119.97	122.90
3	A	903	NAG	C2-N2-C7	-2.18	119.98	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	905	CO3	3	0

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(Å²)	Q<0.9
1	A	638/654 (97%)	0.03	22 (3%)	48	34	45, 81, 127, 200	0
1	B	639/654 (97%)	0.62	64 (10%)	14	10	39, 106, 184, 200	1 (0%)
2	C	515/693 (74%)	0.76	52 (10%)	14	10	70, 127, 182, 200	2 (0%)
2	D	487/693 (70%)	0.63	33 (6%)	25	17	68, 150, 199, 200	1 (0%)
All	All	2279/2694 (84%)	0.49	171 (7%)	22	15	39, 111, 185, 200	4 (0%)

The worst 5 of 171 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	752	ASP	6.3
2	C	189	SER	5.1
1	B	235	ALA	4.8
1	B	264	PHE	4.8
2	D	631	PHE	4.6

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 monosaccharides 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. 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	NAG	B	903	14/15	0.53	0.23	154,154,154,154	0
3	NAG	A	903	14/15	0.62	0.27	134,134,134,134	0
6	CO3	D	905	4/4	0.74	0.12	163,163,163,163	0
5	FE	D	901	1/1	0.94	0.06	128,128,128,128	0
6	CO3	C	905	4/4	0.95	0.06	78,78,78,78	0
5	FE	C	901	1/1	0.98	0.05	98,98,98,98	0
4	CA	B	900	1/1	0.98	0.04	79,79,79,79	0
4	CA	A	900	1/1	0.99	0.07	59,59,59,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.