



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:13 PM EDT

PDB ID : 3S9L / pdb_00003s9l
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)

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

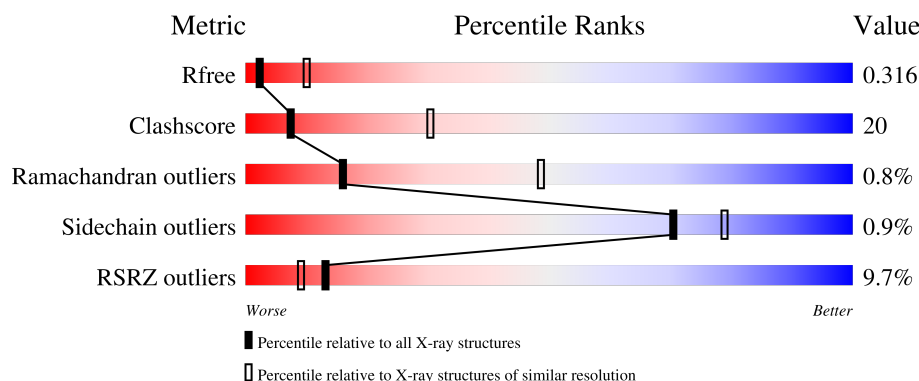
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

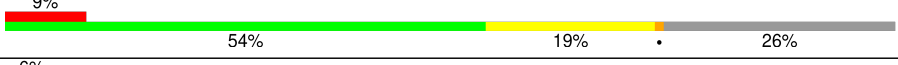
The reported resolution of this entry is 3.22 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (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 $\leq 5\%$. 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	654	
1	B	654	
2	C	693	
2	D	693	

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	C	N	O	S	0	0	0
			3650	2275	615	725	35			
2	D	487	Total	C	N	O	S	0	0	0
			3274	1997	569	675	33			

There are 38 discrepancies between the modelled and reference sequences:

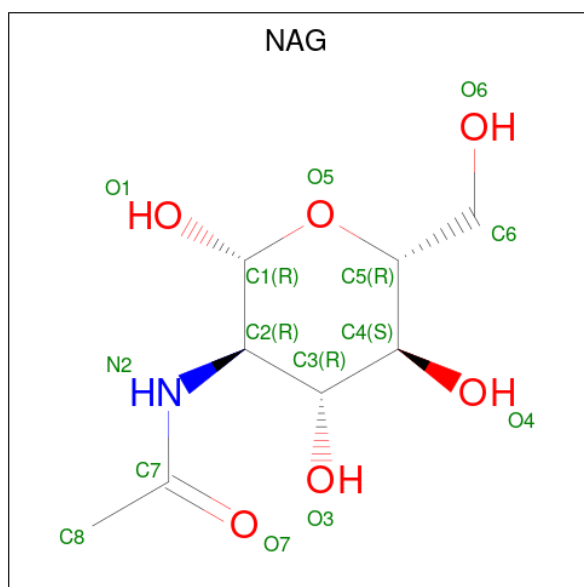
Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	VAL	-	expression tag	UNP P02787
C	-12	PRO	-	expression tag	UNP P02787
C	-11	ASP	-	expression tag	UNP P02787
C	-10	LYS	-	expression tag	UNP P02787
C	-9	HIS	-	expression tag	UNP P02787
C	-8	HIS	-	expression tag	UNP P02787
C	-7	HIS	-	expression tag	UNP 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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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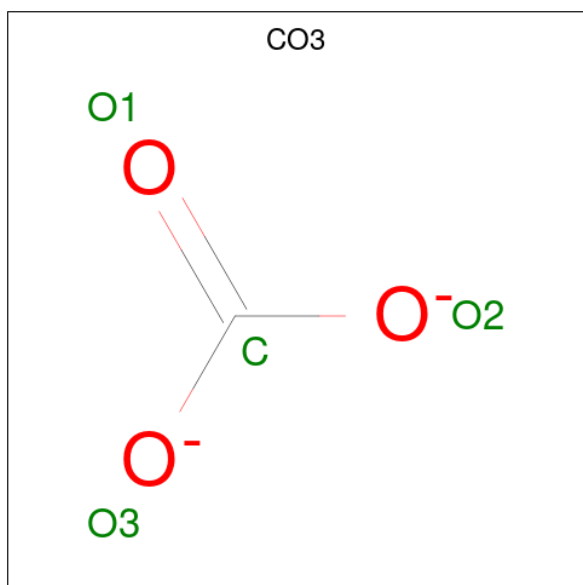
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 6 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).

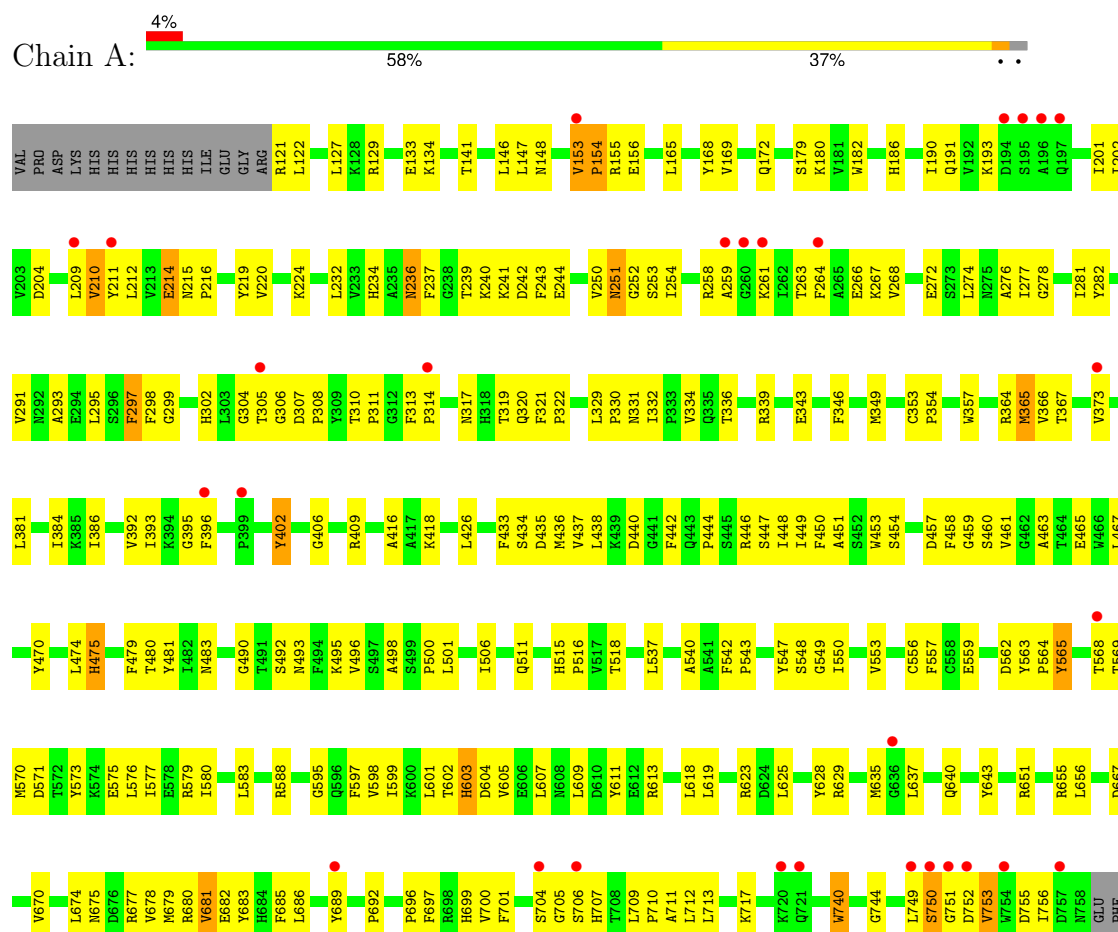


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			4	1	3		
6	D	1	Total	C	O	0	0
			4	1	3		

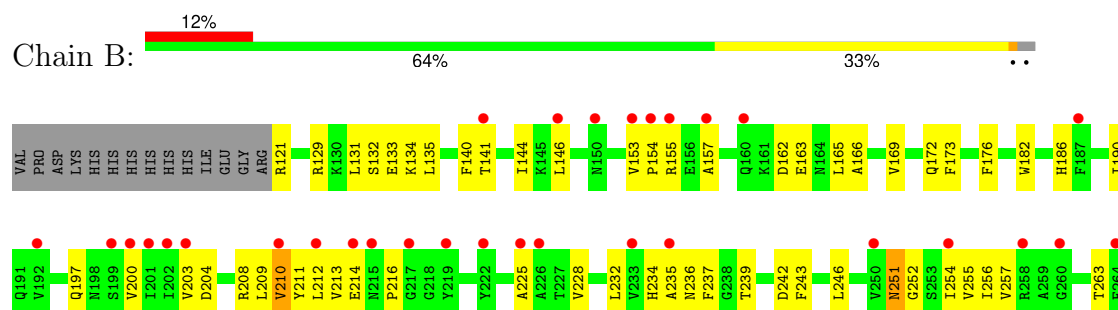
3 Residue-property plots

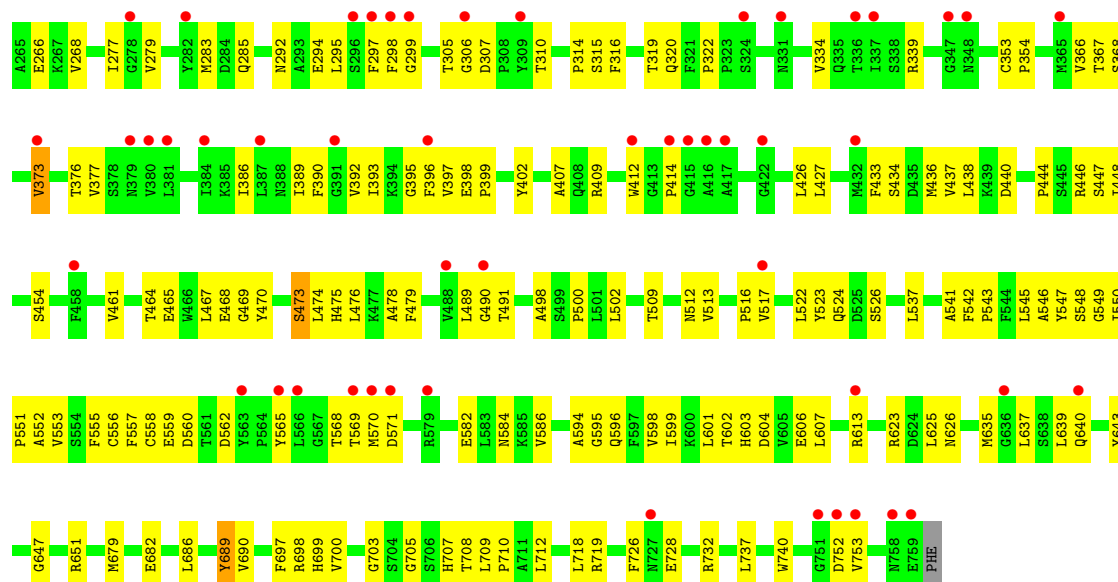
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

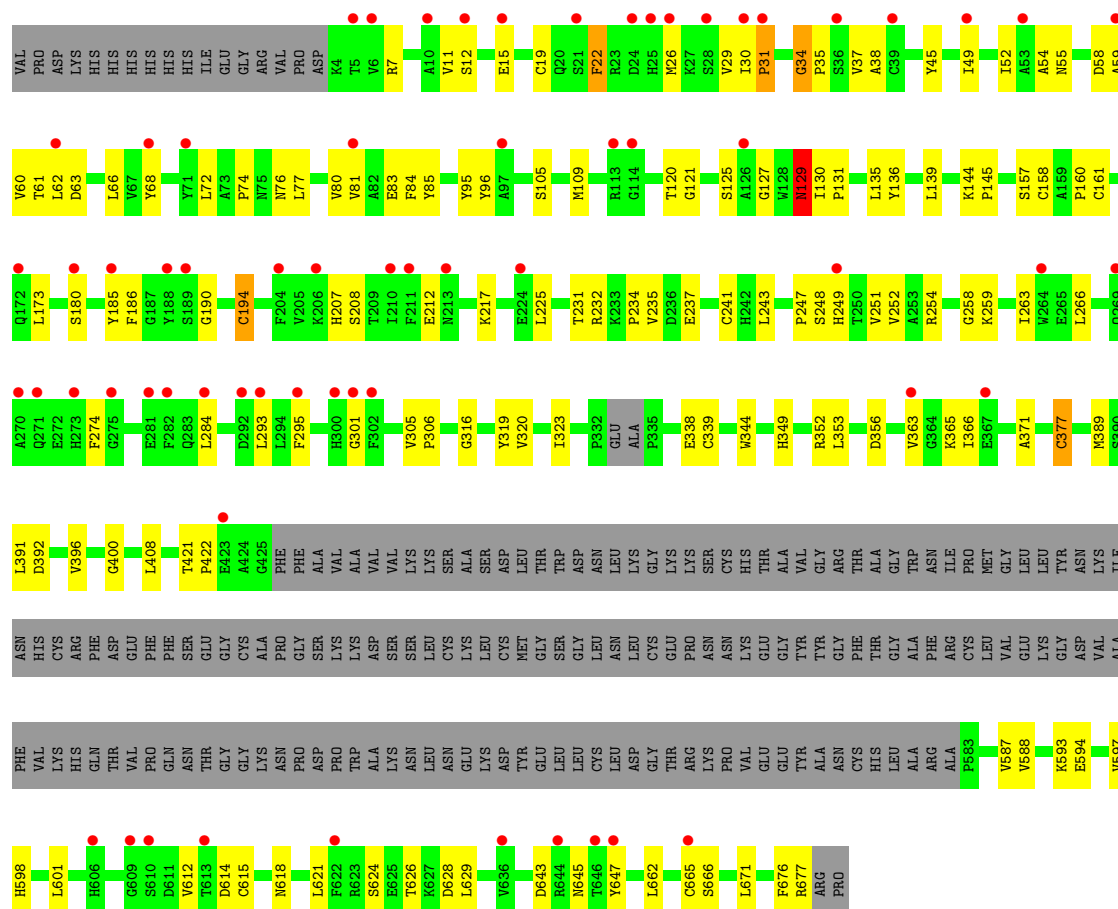


• Molecule 1: Transferrin receptor protein 1

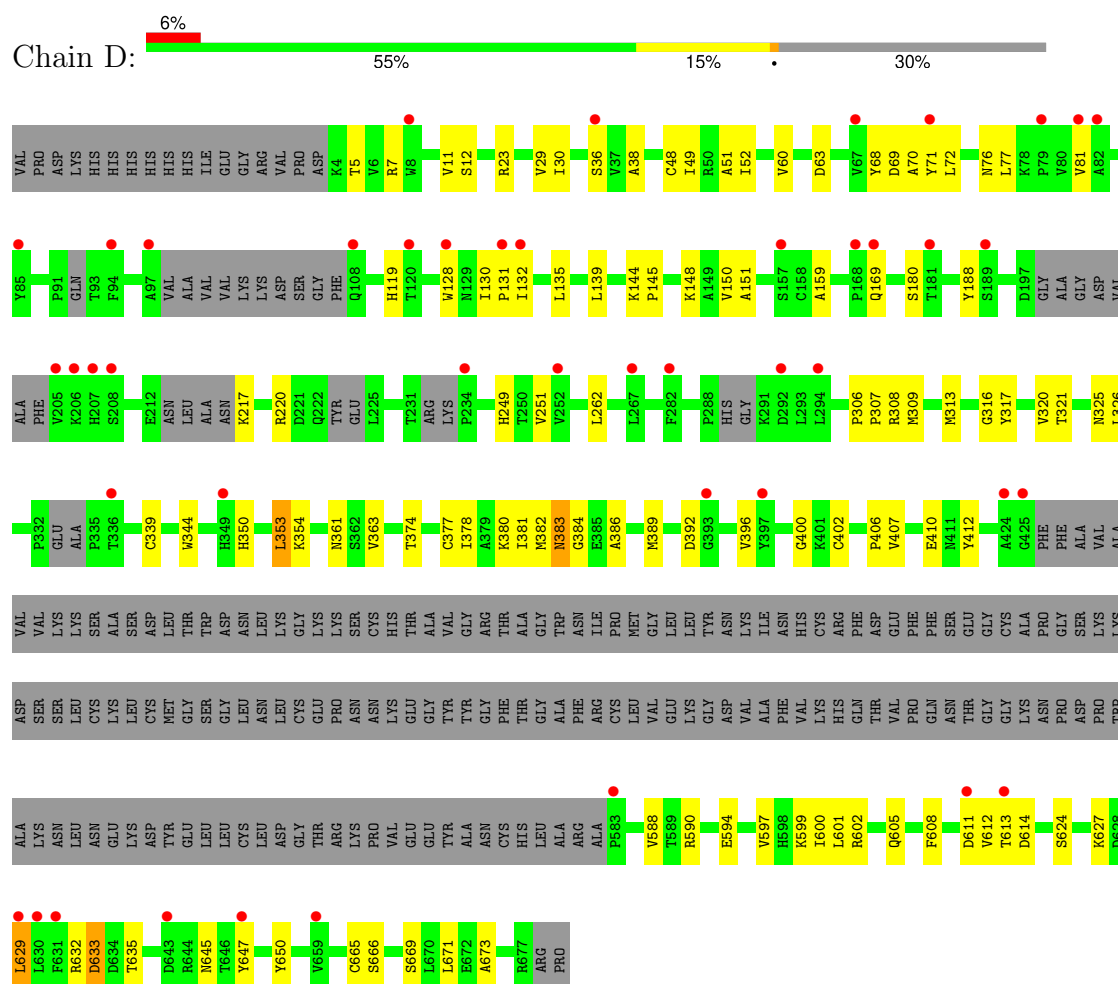




• Molecule 2: Serotransferrin



• Molecule 2: Serotransferrin



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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: CA, NAG, 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	0.52	0/5068	0.94	13/6897 (0.2%)
1	B	0.50	0/4916	0.89	6/6718 (0.1%)
2	C	0.42	0/3725	0.85	4/5095 (0.1%)
2	D	0.39	0/3327	0.82	3/4546 (0.1%)
All	All	0.47	0/17036	0.88	26/23256 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	MET	N-CA-C	7.09	119.01	111.28
2	D	353	LEU	N-CA-C	-6.85	104.56	113.12
1	B	752	ASP	CB-CA-C	-6.72	108.81	116.54
1	B	557	PHE	N-CA-C	-6.63	101.47	110.68
1	A	603	HIS	N-CA-C	6.49	118.93	111.02
1	A	557	PHE	N-CA-C	-6.46	101.70	110.68
2	C	621	LEU	N-CA-C	6.09	118.89	111.82
2	C	129	ASN	N-CA-C	5.92	117.40	111.07
1	B	396	PHE	N-CA-C	5.66	117.53	111.36
1	A	740	TRP	CA-C-N	5.64	127.84	120.28
1	A	740	TRP	C-N-CA	5.64	127.84	120.28
1	A	214	GLU	N-CA-C	5.48	116.85	108.52
1	B	373	VAL	N-CA-C	5.40	116.95	109.45
2	C	194	CYS	N-CA-C	-5.39	106.75	113.38
1	B	689	TYR	N-CA-C	5.37	117.55	111.11
2	D	354	LYS	N-CA-C	-5.33	105.39	111.14
2	D	633	ASP	N-CA-C	5.31	117.07	111.28
1	A	755	ASP	N-CA-C	5.28	117.04	111.28
1	A	402	TYR	N-CA-C	5.21	117.00	108.76
1	A	689	TYR	N-CA-C	5.15	116.89	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	473	SER	N-CA-C	5.12	116.94	111.36
2	C	22	PHE	N-CA-C	-5.08	106.58	112.89
1	A	236	ASN	CB-CA-C	-5.07	110.33	117.23
1	A	753	VAL	N-CA-C	5.07	116.95	111.58
1	A	153	VAL	CB-CA-C	-5.04	109.00	114.35
1	A	569	THR	N-CA-C	-5.03	106.98	113.01

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	254	0
1	B	4800	0	4434	188	0
2	C	3650	0	3184	125	0
2	D	3274	0	2660	89	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
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	648	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.

All (648) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.19
1:A:677:ARG:NH1	1:A:751:GLY:HA2	1.63	1.12
1:B:412:TRP:CH2	1:B:569:THR:HG23	1.86	1.10
1:A:237:PHE:HB3	1:A:261:LYS:CB	1.81	1.09
1:A:210:VAL:HG12	1:A:211:TYR:H	1.22	1.04
2:C:58:ASP:HB3	2:C:259:LYS:HZ3	1.18	1.03
1:A:306:GLY:HA2	1:A:461:VAL:HA	1.04	1.03
1:A:677:ARG:NH1	1:A:751:GLY:CA	2.22	1.03
2:C:30:ILE:HG23	2:C:31:PRO:HA	1.40	0.99
1:B:489:LEU:CD1	1:B:558:CYS:SG	2.52	0.98
2:D:410:GLU:OE1	2:D:632:ARG:HB2	1.62	0.98
2:C:58:ASP:HB3	2:C:259:LYS:NZ	1.82	0.95
1:B:412:TRP:CH2	1:B:569:THR:CG2	2.46	0.94
1:B:306:GLY:HA2	1:B:461:VAL:HA	1.50	0.94
2:D:188:TYR:CZ	6:D:905:CO3:O2	2.21	0.93
1:A:153:VAL:CB	1:A:154:PRO:HD3	1.97	0.93
2:C:58:ASP:CG	2:C:259:LYS:NZ	2.26	0.92
2:C:30:ILE:CG2	2:C:31:PRO:HA	1.99	0.92
1:A:306:GLY:HA2	1:A:461:VAL:CA	1.98	0.92
1:A:677:ARG:HH11	1:A:751:GLY:HA2	1.32	0.91
1:B:640:GLN:HA	1:B:643:TYR:HD1	1.34	0.91
1:A:599:ILE:O	1:A:603:HIS:HB2	1.71	0.90
1:A:704:SER:O	1:A:707:HIS:CE1	2.25	0.90
1:A:259:ALA:HA	1:A:267:LYS:HE3	1.54	0.90
1:B:155:ARG:NH2	1:B:409:ARG:O	2.05	0.90
2:C:30:ILE:CG2	2:C:31:PRO:CA	2.50	0.89
1:B:153:VAL:CB	1:B:154:PRO:HD3	2.02	0.87
1:A:251:ASN:O	1:A:251:ASN:ND2	2.07	0.87
1:B:412:TRP:HZ3	1:B:569:THR:HG23	1.03	0.86
2:C:105:SER:HB2	2:C:232:ARG:HH22	1.38	0.86
1:A:565:TYR:HB3	1:A:568:THR:OG1	1.76	0.86
1:A:237:PHE:CB	1:A:261:LYS:CB	2.54	0.85
1:A:251:ASN:C	1:A:251:ASN:HD22	1.83	0.84
2:C:58:ASP:CB	2:C:259:LYS:NZ	2.40	0.84
1:B:155:ARG:HH12	1:B:165:LEU:HD22	1.44	0.82
2:C:30:ILE:HG23	2:C:31:PRO:CA	2.08	0.82
1:A:237:PHE:CG	1:A:261:LYS:CB	2.62	0.82
2:C:49:ILE:HG23	2:C:77:LEU:HD12	1.60	0.82
1:A:306:GLY:CA	1:A:461:VAL:HA	2.00	0.82
2:C:30:ILE:CG2	2:C:31:PRO:HB3	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:HIS:ND1	1:B:476:LEU:HG	1.96	0.81
1:A:599:ILE:O	1:A:603:HIS:CB	2.29	0.81
1:B:412:TRP:HZ3	1:B:569:THR:CG2	1.72	0.80
2:D:128:TRP:CH2	2:D:150:VAL:HG21	2.15	0.80
1:B:479:PHE:HB3	1:B:679:MET:HE3	1.64	0.80
1:A:193:LYS:HD2	1:A:219:TYR:HB3	1.63	0.80
1:B:412:TRP:CZ3	1:B:569:THR:HG22	2.17	0.79
2:C:30:ILE:HG22	2:C:31:PRO:HB3	1.64	0.78
1:A:210:VAL:HG12	1:A:211:TYR:N	1.99	0.78
1:B:565:TYR:HB3	1:B:568:THR:OG1	1.84	0.77
2:C:83:GLU:HG2	2:C:249:HIS:O	1.82	0.77
2:C:30:ILE:HG22	2:C:31:PRO:CB	2.15	0.77
2:C:624:SER:HB3	2:C:629:LEU:HD13	1.64	0.76
1:A:204:ASP:HB2	1:A:209:LEU:CB	2.16	0.75
1:A:677:ARG:NH1	1:A:751:GLY:HA3	2.01	0.75
1:A:542:PHE:HB3	1:A:543:PRO:HD3	1.68	0.75
2:D:52:ILE:HD11	2:D:60:VAL:HG12	1.69	0.75
1:A:263:THR:OG1	1:A:266:GLU:HG3	1.87	0.75
1:B:436:MET:HA	1:B:440:ASP:HB2	1.69	0.75
1:A:565:TYR:HB3	1:A:570:MET:HB2	1.69	0.74
2:D:68:TYR:O	2:D:72:LEU:HG	1.86	0.74
2:D:412:TYR:CE1	2:D:632:ARG:CD	2.70	0.74
2:D:188:TYR:OH	6:D:905:CO3:O2	2.06	0.74
1:B:172:GLN:HG3	1:B:176:PHE:CZ	2.23	0.74
1:A:201:ILE:HG22	1:A:212:LEU:HA	1.69	0.74
2:C:37:VAL:HG22	2:C:266:LEU:HD21	1.69	0.74
1:A:667:ASP:HB3	1:A:670:VAL:HG12	1.69	0.73
1:B:295:LEU:HD21	1:B:568:THR:HG21	1.69	0.73
1:B:263:THR:OG1	1:B:266:GLU:HG3	1.86	0.73
2:C:258:GLY:O	2:C:259:LYS:HG2	1.88	0.73
2:D:632:ARG:HB2	2:D:635:THR:OG1	1.87	0.73
2:D:412:TYR:OH	2:D:632:ARG:CD	2.37	0.73
1:A:386:ILE:HG23	1:A:454:SER:HB3	1.71	0.73
1:B:626:ASN:C	1:B:626:ASN:HD22	1.95	0.72
2:C:30:ILE:CG2	2:C:31:PRO:CB	2.67	0.72
1:A:263:THR:HG1	1:A:266:GLU:HG3	1.55	0.72
1:A:278:GLY:HA2	1:A:332:ILE:HG23	1.72	0.72
1:B:134:LYS:NZ	1:B:440:ASP:OD2	2.18	0.72
1:A:740:TRP:O	1:A:744:GLY:N	2.23	0.71
1:B:251:ASN:C	1:B:251:ASN:HD22	1.96	0.71
1:B:753:VAL:HG12	1:B:753:VAL:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:410:GLU:OE1	2:D:632:ARG:CB	2.38	0.71
1:B:395:GLY:O	1:B:399:PRO:HG3	1.90	0.71
1:A:756:ILE:O	1:A:756:ILE:HG13	1.91	0.70
1:A:433:PHE:HE1	1:A:599:ILE:HD11	1.57	0.70
1:A:168:TYR:CE1	1:A:172:GLN:NE2	2.59	0.70
2:C:234:PRO:HD2	2:C:237:GLU:OE1	1.91	0.70
1:A:155:ARG:HD2	1:A:409:ARG:O	1.91	0.70
2:C:377:CYS:HB3	2:C:389:MET:SD	2.32	0.70
1:A:629:ARG:NH2	2:C:618:ASN:OD1	2.26	0.69
1:B:549:GLY:HA3	1:B:686:LEU:HD11	1.73	0.69
1:A:180:LYS:HB3	1:A:392:VAL:HG12	1.73	0.69
2:C:58:ASP:CB	2:C:259:LYS:HZ3	1.95	0.69
2:C:30:ILE:HG22	2:C:31:PRO:CA	2.22	0.69
2:C:7:ARG:HA	2:C:38:ALA:HB3	1.75	0.69
1:B:386:ILE:HG23	1:B:454:SER:HB3	1.73	0.69
1:A:565:TYR:O	1:A:571:ASP:HB2	1.93	0.68
2:C:135:LEU:O	2:C:139:LEU:HG	1.93	0.68
2:D:63:ASP:OD1	2:D:249:HIS:NE2	2.27	0.68
1:B:235:ALA:HB2	1:B:255:VAL:HB	1.76	0.67
2:C:96:TYR:HB2	2:C:207:HIS:CD2	2.29	0.67
1:A:565:TYR:CD2	1:A:570:MET:SD	2.88	0.67
1:A:479:PHE:HB3	1:A:679:MET:HE3	1.77	0.67
2:D:63:ASP:OD1	2:D:249:HIS:CE1	2.48	0.67
2:D:188:TYR:CE1	6:D:905:CO3:O2	2.48	0.67
1:A:168:TYR:O	1:A:172:GLN:HG2	1.95	0.66
1:A:180:LYS:HB3	1:A:392:VAL:CG1	2.25	0.66
1:B:172:GLN:HG2	1:B:427:LEU:HD22	1.76	0.66
1:B:305:THR:HG21	1:B:543:PRO:HG3	1.76	0.66
1:B:509:THR:HG23	1:B:596:GLN:HE21	1.62	0.65
2:D:7:ARG:HA	2:D:38:ALA:HB3	1.79	0.65
2:C:344:TRP:HZ3	2:C:601:LEU:HD21	1.62	0.65
1:A:210:VAL:CG1	1:A:211:TYR:H	2.06	0.65
1:B:200:VAL:HG13	1:B:213:VAL:HB	1.78	0.65
1:A:252:GLY:HA2	1:A:277:ILE:HD11	1.78	0.64
2:C:208:SER:O	2:C:212:GLU:HG3	1.97	0.64
1:A:623:ARG:CZ	2:C:363:VAL:HG22	2.26	0.64
1:B:640:GLN:HA	1:B:643:TYR:CD1	2.24	0.64
1:A:565:TYR:CE2	1:A:570:MET:SD	2.91	0.64
1:A:121:ARG:NH1	1:A:121:ARG:HB3	2.13	0.64
2:C:96:TYR:HB2	2:C:207:HIS:HD2	1.62	0.64
2:D:12:SER:HB2	2:D:180:SER:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ARG:O	1:A:655:ARG:HG3	1.98	0.63
2:C:34:GLY:H	2:C:35:PRO:CD	2.11	0.63
2:D:262:LEU:O	2:D:262:LEU:HD23	1.99	0.63
1:A:307:ASP:OD1	1:A:308:PRO:N	2.32	0.63
1:B:285:GLN:HG3	1:B:339:ARG:NH1	2.13	0.63
1:A:239:THR:HB	1:A:242:ASP:OD1	1.99	0.63
1:A:579:ARG:HH11	1:A:579:ARG:HB3	1.64	0.63
1:B:479:PHE:HE1	1:B:601:LEU:HB3	1.65	0.62
1:A:579:ARG:HB3	1:A:579:ARG:NH1	2.15	0.62
1:A:237:PHE:CD2	1:A:261:LYS:CB	2.83	0.61
1:B:541:ALA:HB1	1:B:552:ALA:HB1	1.82	0.61
2:D:363:VAL:HG12	2:D:363:VAL:O	2.00	0.61
1:A:146:LEU:O	1:A:146:LEU:HD23	1.99	0.61
1:A:305:THR:HG21	1:A:543:PRO:HG3	1.83	0.61
1:A:493:ASN:HD21	1:A:495:LYS:HE3	1.65	0.61
2:D:217:LYS:HA	2:D:220:ARG:HE	1.66	0.61
1:B:595:GLY:O	1:B:599:ILE:HG13	2.01	0.61
2:C:52:ILE:O	2:C:254:ARG:HD3	2.01	0.61
1:A:182:TRP:CH2	1:A:392:VAL:HB	2.36	0.61
2:D:412:TYR:CZ	2:D:632:ARG:CD	2.84	0.61
1:B:446:ARG:H	1:B:602:THR:HG23	1.66	0.61
1:B:392:VAL:HG23	1:B:448:ILE:O	2.01	0.60
2:C:344:TRP:CZ3	2:C:601:LEU:HD21	2.36	0.60
2:D:306:PRO:HG2	2:D:673:ALA:HA	1.82	0.60
1:A:595:GLY:O	1:A:599:ILE:HG12	2.01	0.60
1:B:140:PHE:O	1:B:144:ILE:HG13	2.00	0.60
1:B:314:PRO:HG3	1:B:469:GLY:HA2	1.83	0.60
1:A:155:ARG:O	1:A:156:GLU:C	2.44	0.60
1:B:568:THR:OG1	1:B:570:MET:HG2	2.00	0.60
1:A:418:LYS:HE2	1:A:457:ASP:OD1	2.01	0.60
1:B:210:VAL:HG12	1:B:211:TYR:H	1.67	0.60
2:C:371:ALA:HB3	2:C:377:CYS:SG	2.42	0.60
1:A:148:ASN:HD21	1:A:416:ALA:HB2	1.65	0.60
1:B:565:TYR:HB3	1:B:568:THR:HG1	1.67	0.60
1:A:202:ILE:O	1:A:210:VAL:HB	2.02	0.59
2:C:105:SER:HB2	2:C:232:ARG:NH2	2.15	0.59
2:C:662:LEU:HD23	2:C:662:LEU:O	2.02	0.59
1:B:502:LEU:HD13	1:B:553:VAL:HB	1.84	0.59
1:A:366:VAL:HG12	1:A:367:THR:N	2.18	0.59
1:A:640:GLN:HA	1:A:643:TYR:CD1	2.38	0.59
1:A:680:ARG:O	1:A:681:VAL:C	2.46	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:120:THR:OG1	2:C:127:GLY:HA3	2.03	0.59
1:B:626:ASN:O	1:B:626:ASN:ND2	2.25	0.59
1:B:295:LEU:HD21	1:B:568:THR:CG2	2.33	0.58
1:A:295:LEU:HD21	1:A:568:THR:HB	1.84	0.58
2:C:217:LYS:O	2:C:217:LYS:HD3	2.03	0.58
1:A:562:ASP:N	1:A:562:ASP:OD2	2.37	0.58
1:B:172:GLN:HG3	1:B:176:PHE:CE2	2.38	0.58
1:A:339:ARG:O	1:A:343:GLU:HG3	2.03	0.58
1:A:446:ARG:NE	1:A:607:LEU:HD21	2.19	0.58
1:A:685:PHE:HB3	1:A:699:HIS:CE1	2.39	0.58
1:B:165:LEU:O	1:B:169:VAL:HG23	2.04	0.58
1:B:153:VAL:CB	1:B:154:PRO:CD	2.79	0.58
2:C:130:ILE:N	2:C:131:PRO:HD2	2.18	0.58
2:D:23:ARG:HD2	2:D:23:ARG:C	2.29	0.58
1:A:433:PHE:HE1	1:A:599:ILE:CD1	2.16	0.57
1:B:562:ASP:OD2	1:B:562:ASP:N	2.37	0.57
1:A:656:LEU:HD22	1:A:749:LEU:HD11	1.87	0.57
1:A:640:GLN:HA	1:A:643:TYR:HD1	1.68	0.57
2:C:258:GLY:O	2:C:259:LYS:CG	2.53	0.57
1:A:232:LEU:HD13	1:A:373:VAL:HG21	1.87	0.57
2:C:160:PRO:O	2:C:161:CYS:HB2	2.04	0.57
2:C:231:THR:HG22	2:C:232:ARG:H	1.69	0.57
1:A:147:LEU:HD22	1:A:165:LEU:HD11	1.86	0.57
1:A:565:TYR:CB	1:A:568:THR:OG1	2.51	0.57
1:B:155:ARG:NH1	1:B:165:LEU:HD22	2.18	0.57
1:B:753:VAL:O	1:B:753:VAL:CG1	2.53	0.57
1:A:628:TYR:OH	1:A:717:LYS:HG2	2.05	0.56
2:C:49:ILE:HG23	2:C:77:LEU:CD1	2.31	0.56
1:A:500:PRO:HB3	1:A:613:ARG:HG3	1.86	0.56
1:A:667:ASP:OD1	2:C:74:PRO:HD3	2.06	0.56
1:A:704:SER:O	1:A:707:HIS:NE2	2.38	0.56
1:A:498:ALA:HB2	1:A:553:VAL:HA	1.88	0.56
1:B:623:ARG:HD3	2:D:363:VAL:HG22	1.88	0.56
2:D:130:ILE:N	2:D:131:PRO:HD2	2.21	0.56
1:A:467:LEU:HD22	1:A:548:SER:OG	2.05	0.56
2:C:12:SER:HB2	2:C:180:SER:HB2	1.87	0.56
1:A:250:VAL:HG12	1:A:250:VAL:O	2.04	0.56
1:B:414:PRO:HG2	1:B:571:ASP:O	2.06	0.56
2:C:129:ASN:N	2:C:129:ASN:HD22	2.02	0.56
2:C:157:SER:N	2:C:173:LEU:HD13	2.20	0.56
2:C:338:GLU:O	2:C:339:CYS:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ALA:HB3	1:B:426:LEU:HD22	1.88	0.56
2:C:391:LEU:HD12	2:C:588:VAL:HG21	1.87	0.56
1:A:568:THR:OG1	1:A:570:MET:HB2	2.06	0.56
2:D:412:TYR:HE1	2:D:632:ARG:CD	2.17	0.56
1:A:297:PHE:N	1:A:297:PHE:CD2	2.72	0.56
1:A:543:PRO:O	1:A:547:TYR:HB3	2.05	0.56
1:A:549:GLY:HA3	1:A:686:LEU:HD11	1.88	0.55
2:D:599:LYS:HZ2	2:D:600:ILE:HD13	1.71	0.55
1:B:234:HIS:HA	1:B:256:ILE:CG2	2.37	0.55
1:B:214:GLU:O	1:B:216:PRO:HD3	2.06	0.55
1:A:302:HIS:CE1	1:A:304:GLY:HA3	2.42	0.55
1:A:680:ARG:O	1:A:683:TYR:N	2.40	0.55
1:B:647:GLY:O	1:B:651:ARG:HG3	2.06	0.55
2:D:383:ASN:N	2:D:383:ASN:HD22	2.04	0.55
1:A:191:GLN:HB2	1:A:381:LEU:HD23	1.89	0.55
2:C:59:ALA:HB2	2:C:263:ILE:HD13	1.88	0.55
2:C:29:VAL:O	2:C:29:VAL:HG22	2.07	0.55
2:C:62:LEU:HD23	2:C:252:VAL:HG22	1.87	0.55
2:D:217:LYS:O	2:D:217:LYS:HD3	2.07	0.55
1:A:127:LEU:HD22	1:A:442:PHE:CD1	2.42	0.55
2:D:69:ASP:HA	2:D:72:LEU:HD12	1.89	0.55
1:B:157:ALA:HA	1:B:162:ASP:OD1	2.06	0.55
1:B:366:VAL:HG12	1:B:367:THR:N	2.21	0.54
2:C:671:LEU:HD13	2:C:671:LEU:O	2.06	0.54
1:A:635:MET:O	1:A:637:LEU:N	2.39	0.54
1:A:700:VAL:HB	1:A:709:LEU:HD13	1.89	0.54
1:B:251:ASN:O	1:B:251:ASN:ND2	2.28	0.54
1:A:278:GLY:HA2	1:A:332:ILE:CG2	2.37	0.54
1:B:203:VAL:HG12	1:B:208:ARG:HA	1.88	0.54
2:C:63:ASP:OD1	2:C:249:HIS:CD2	2.59	0.54
1:A:129:ARG:O	1:A:133:GLU:HG3	2.08	0.54
1:B:479:PHE:O	1:B:551:PRO:HD2	2.08	0.54
1:A:302:HIS:CE1	1:A:308:PRO:HB3	2.42	0.54
1:A:122:LEU:N	1:A:122:LEU:HD12	2.23	0.54
1:A:224:LYS:HD2	1:A:331:ASN:C	2.33	0.54
1:A:295:LEU:HD21	1:A:568:THR:CB	2.37	0.54
1:A:297:PHE:H	1:A:297:PHE:HD2	1.54	0.54
1:A:436:MET:HA	1:A:440:ASP:HB2	1.90	0.54
1:A:677:ARG:CZ	1:A:751:GLY:HA2	2.35	0.54
1:A:202:ILE:HG22	1:A:210:VAL:HG21	1.90	0.54
2:D:597:VAL:HG13	2:D:601:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:68:TYR:O	2:C:72:LEU:HG	2.07	0.53
2:D:29:VAL:HG23	2:D:30:ILE:HG12	1.89	0.53
1:B:690:VAL:HG23	1:B:698:ARG:HG2	1.89	0.53
1:A:305:THR:CG2	1:A:543:PRO:HG3	2.38	0.53
1:B:498:ALA:HB2	1:B:553:VAL:HA	1.89	0.53
1:B:542:PHE:HB3	1:B:543:PRO:HD3	1.90	0.53
1:A:565:TYR:HB3	1:A:570:MET:CB	2.39	0.53
1:B:582:GLU:CD	1:B:582:GLU:H	2.16	0.53
1:B:626:ASN:C	1:B:626:ASN:ND2	2.65	0.53
1:B:210:VAL:HG12	1:B:211:TYR:N	2.24	0.53
1:A:474:LEU:O	1:A:475:HIS:C	2.51	0.53
1:A:190:ILE:HB	1:A:458:PHE:CE2	2.43	0.53
1:B:232:LEU:HD22	1:B:373:VAL:HG11	1.91	0.53
2:C:593:LYS:O	2:C:597:VAL:HG23	2.09	0.53
2:D:344:TRP:HZ3	2:D:601:LEU:HD21	1.74	0.53
1:A:224:LYS:HD2	1:A:331:ASN:O	2.08	0.52
1:B:146:LEU:HD23	1:B:146:LEU:O	2.09	0.52
1:B:392:VAL:HG22	1:B:393:ILE:N	2.24	0.52
2:C:258:GLY:C	2:C:259:LYS:HG2	2.33	0.52
1:A:677:ARG:HH11	1:A:751:GLY:CA	2.06	0.52
1:B:434:SER:O	1:B:438:LEU:HD23	2.10	0.52
2:C:30:ILE:HG23	2:C:31:PRO:CB	2.38	0.52
2:D:308:ARG:HB2	2:D:669:SER:HB2	1.91	0.52
2:D:381:ILE:HA	2:D:386:ALA:O	2.10	0.52
1:B:446:ARG:HE	1:B:607:LEU:HD21	1.73	0.52
2:C:676:PHE:HD1	2:C:677:ARG:HG3	1.74	0.52
1:B:155:ARG:HH12	1:B:165:LEU:CD2	2.19	0.52
1:B:489:LEU:HD12	1:B:556:CYS:SG	2.50	0.52
2:D:361:ASN:HB3	2:D:608:PHE:CZ	2.44	0.52
1:A:153:VAL:CB	1:A:154:PRO:CD	2.82	0.52
2:C:45:TYR:CE2	2:C:66:LEU:HD22	2.44	0.52
1:B:283:MET:HE2	1:B:297:PHE:CD2	2.45	0.52
1:A:317:ASN:HA	1:A:321:PHE:CE1	2.45	0.52
1:A:619:LEU:O	1:A:619:LEU:HD23	2.10	0.52
2:D:23:ARG:HD2	2:D:23:ARG:O	2.09	0.52
2:D:400:GLY:HA3	2:D:647:TYR:HB3	1.90	0.52
1:A:193:LYS:NZ	1:A:216:PRO:O	2.42	0.51
1:A:297:PHE:N	1:A:297:PHE:HD2	2.07	0.51
1:B:376:THR:HG23	1:B:376:THR:O	2.09	0.51
1:A:446:ARG:HE	1:A:607:LEU:HD21	1.75	0.51
1:A:182:TRP:HH2	1:A:392:VAL:HB	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:611:ASP:OD1	2:D:612:VAL:N	2.43	0.51
1:B:397:VAL:C	1:B:399:PRO:HD3	2.35	0.51
1:B:489:LEU:HB2	1:B:558:CYS:HA	1.91	0.51
2:C:293:LEU:O	2:C:295:PHE:N	2.43	0.51
1:A:480:THR:HG22	1:A:481:TYR:N	2.25	0.51
2:C:63:ASP:HA	2:C:249:HIS:CD2	2.46	0.51
2:D:321:THR:HG22	2:D:325:ASN:ND2	2.25	0.51
1:B:474:LEU:O	1:B:475:HIS:C	2.53	0.51
1:B:708:THR:HB	1:B:710:PRO:HD2	1.91	0.51
1:A:186:HIS:CE1	1:A:465:GLU:HB3	2.46	0.51
2:D:309:MET:HG3	2:D:313:MET:CG	2.41	0.51
1:A:740:TRP:HA	1:A:740:TRP:CE3	2.46	0.51
1:A:474:LEU:HD13	1:A:550:ILE:HD11	1.93	0.50
1:B:232:LEU:HB2	1:B:373:VAL:CG2	2.42	0.50
2:C:37:VAL:CG2	2:C:266:LEU:HD21	2.38	0.50
2:C:319:TYR:O	2:C:323:ILE:HG13	2.11	0.50
2:D:378:ILE:O	2:D:382:MET:HG3	2.10	0.50
1:A:346:PHE:O	1:A:364:ARG:HG3	2.11	0.50
1:A:395:GLY:HA2	1:A:444:PRO:HG2	1.94	0.50
1:A:298:PHE:HE2	1:A:457:ASP:HB3	1.75	0.50
1:B:234:HIS:HA	1:B:256:ILE:HG23	1.92	0.50
2:D:49:ILE:HG23	2:D:77:LEU:HD12	1.92	0.50
1:A:191:GLN:CB	1:A:381:LEU:HD23	2.41	0.50
1:B:204:ASP:HB2	1:B:209:LEU:CB	2.42	0.50
2:C:136:TYR:HA	2:C:139:LEU:HD12	1.93	0.50
1:A:675:ASN:O	1:A:679:MET:HG3	2.12	0.50
1:A:751:GLY:O	1:A:752:ASP:OD1	2.30	0.50
1:B:712:LEU:C	1:B:712:LEU:HD23	2.37	0.50
1:B:728:GLU:HG2	1:B:732:ARG:HE	1.77	0.50
1:A:579:ARG:HH11	1:A:579:ARG:CB	2.25	0.50
1:B:412:TRP:HH2	1:B:569:THR:CG2	2.21	0.50
1:B:512:ASN:ND2	1:B:596:GLN:OE1	2.45	0.50
1:B:635:MET:O	1:B:637:LEU:N	2.40	0.50
2:D:71:TYR:HA	2:D:77:LEU:H	1.77	0.50
1:A:272:GLU:HG3	1:A:332:ILE:HD12	1.94	0.50
1:B:236:ASN:ND2	1:B:237:PHE:H	2.10	0.50
2:C:11:VAL:O	2:C:12:SER:HB3	2.12	0.50
1:A:623:ARG:NH1	2:C:363:VAL:HG22	2.26	0.49
1:B:474:LEU:HD13	1:B:550:ILE:HD11	1.93	0.49
2:D:377:CYS:HB3	2:D:389:MET:SD	2.52	0.49
1:B:235:ALA:HB3	1:B:257:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:LEU:HD13	1:B:548:SER:OG	2.13	0.49
2:D:383:ASN:HD22	2:D:384:GLY:N	2.10	0.49
1:B:366:VAL:HG12	1:B:367:THR:H	1.77	0.49
1:B:402:TYR:OH	1:B:474:LEU:HB3	2.12	0.49
1:B:444:PRO:HB2	1:B:602:THR:HG21	1.95	0.49
2:C:109:MET:HE3	2:C:243:LEU:HD21	1.94	0.49
2:D:382:MET:CE	2:D:402:CYS:HB3	2.42	0.49
1:A:751:GLY:C	1:A:752:ASP:OD1	2.56	0.49
1:B:516:PRO:HG3	1:B:586:VAL:HA	1.95	0.49
2:D:128:TRP:CD1	2:D:128:TRP:C	2.91	0.49
2:D:624:SER:HB3	2:D:629:LEU:HD12	1.94	0.49
2:D:128:TRP:CZ2	2:D:150:VAL:HG21	2.48	0.49
1:B:491:THR:OG1	1:B:517:VAL:HG21	2.13	0.48
1:B:705:GLY:HA3	1:B:707:HIS:CE1	2.48	0.48
2:D:383:ASN:HD22	2:D:384:GLY:H	1.59	0.48
1:A:240:LYS:O	1:A:244:GLU:HG3	2.13	0.48
1:B:121:ARG:HB3	1:B:121:ARG:NH1	2.28	0.48
1:B:163:GLU:O	1:B:166:ALA:HB3	2.12	0.48
1:B:295:LEU:CD2	1:B:568:THR:HG21	2.41	0.48
2:C:60:VAL:HG13	2:C:62:LEU:CD2	2.43	0.48
1:A:243:PHE:HB3	1:A:274:LEU:CD1	2.42	0.48
1:A:295:LEU:HD21	1:A:568:THR:HG21	1.96	0.48
2:C:34:GLY:N	2:C:35:PRO:CD	2.75	0.48
2:D:135:LEU:O	2:D:139:LEU:HG	2.13	0.48
1:A:667:ASP:HB3	1:A:670:VAL:CG1	2.40	0.48
1:A:295:LEU:HD21	1:A:568:THR:CG2	2.44	0.48
1:A:433:PHE:O	1:A:437:VAL:HG23	2.13	0.48
1:A:677:ARG:HH12	1:A:751:GLY:HA3	1.76	0.48
1:B:509:THR:HG23	1:B:596:GLN:NE2	2.28	0.48
2:D:128:TRP:CD2	2:D:132:ILE:HG13	2.49	0.48
1:A:268:VAL:HG21	1:A:334:VAL:HG21	1.96	0.48
1:A:706:SER:HA	1:A:711:ALA:HB1	1.95	0.48
1:B:298:PHE:CG	1:B:299:GLY:N	2.82	0.48
2:D:326:LEU:HD23	2:D:326:LEU:O	2.12	0.48
1:A:604:ASP:CG	1:A:605:VAL:H	2.21	0.48
1:B:268:VAL:HG21	1:B:334:VAL:HG21	1.95	0.48
2:D:217:LYS:HA	2:D:220:ARG:NE	2.29	0.48
1:A:272:GLU:HG3	1:A:332:ILE:CD1	2.44	0.48
1:A:537:LEU:H	1:A:537:LEU:HD12	1.78	0.48
1:A:253:SER:N	1:A:277:ILE:HG12	2.29	0.47
1:A:604:ASP:CG	1:A:605:VAL:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:ALA:HB1	1:B:697:PHE:HB3	1.95	0.47
1:A:674:LEU:O	1:A:678:VAL:HG23	2.14	0.47
1:B:307:ASP:N	1:B:461:VAL:HG13	2.30	0.47
1:B:225:ALA:HA	1:B:377:VAL:HB	1.96	0.47
1:A:141:THR:HG22	1:A:583:LEU:HD23	1.96	0.47
2:D:627:LYS:HA	2:D:633:ASP:OD2	2.14	0.47
1:A:402:TYR:HB3	1:A:447:SER:HB2	1.95	0.47
1:A:515:HIS:HB3	1:A:518:THR:O	2.15	0.47
1:A:565:TYR:CD2	1:A:570:MET:HB3	2.50	0.47
1:A:603:HIS:CD2	1:A:603:HIS:C	2.93	0.47
1:B:254:ILE:HD12	1:B:373:VAL:HG23	1.96	0.47
1:A:446:ARG:HB2	1:A:602:THR:HG22	1.97	0.47
1:A:573:TYR:O	1:A:577:ILE:HG22	2.15	0.47
2:C:54:ALA:O	2:C:55:ASN:CG	2.58	0.47
1:B:131:LEU:HD22	1:B:599:ILE:HD11	1.96	0.47
2:D:665:CYS:SG	2:D:666:SER:N	2.88	0.47
1:A:313:PHE:HB2	1:A:314:PRO:HD2	1.97	0.47
1:A:492:SER:OG	1:A:559:GLU:OE2	2.23	0.47
1:B:141:THR:HG22	1:B:584:ASN:HD22	1.80	0.47
1:B:625:LEU:HD23	1:B:639:LEU:HD11	1.97	0.47
1:A:470:TYR:O	1:A:474:LEU:HG	2.15	0.47
2:D:353:LEU:HD23	2:D:353:LEU:O	2.15	0.47
1:A:599:ILE:O	1:A:603:HIS:HB3	2.12	0.46
1:A:651:ARG:NH2	2:C:356:ASP:OD2	2.48	0.46
2:C:96:TYR:H	2:C:207:HIS:HD2	1.64	0.46
1:A:232:LEU:HA	1:A:254:ILE:O	2.15	0.46
2:D:188:TYR:OH	2:D:249:HIS:NE2	2.43	0.46
2:D:632:ARG:HB2	2:D:635:THR:HG1	1.79	0.46
1:A:293:ALA:HB2	1:A:339:ARG:NH2	2.30	0.46
1:A:433:PHE:CE1	1:A:599:ILE:HD11	2.44	0.46
1:B:200:VAL:HG13	1:B:200:VAL:O	2.15	0.46
1:B:235:ALA:HB3	1:B:257:VAL:HG13	1.96	0.46
1:B:367:THR:HG22	1:B:368:SER:N	2.30	0.46
1:B:555:PHE:CZ	1:B:594:ALA:HB2	2.50	0.46
1:A:677:ARG:CZ	1:A:750:SER:O	2.64	0.46
2:C:96:TYR:H	2:C:207:HIS:CD2	2.33	0.46
2:C:109:MET:CE	2:C:243:LEU:HD21	2.45	0.46
2:D:11:VAL:O	2:D:12:SER:HB3	2.15	0.46
1:B:165:LEU:HD23	1:B:409:ARG:HG2	1.97	0.46
2:C:392:ASP:O	2:C:396:VAL:HG23	2.16	0.46
1:A:479:PHE:HE1	1:A:601:LEU:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:316:GLY:O	2:C:320:VAL:HG23	2.16	0.46
2:C:594:GLU:O	2:C:598:HIS:HB2	2.16	0.46
1:A:232:LEU:HB3	1:A:367:THR:HG23	1.98	0.46
1:A:495:LYS:O	1:A:556:CYS:N	2.48	0.46
1:B:292:ASN:HD21	1:B:294:GLU:C	2.24	0.46
1:B:310:THR:OG1	1:B:315:SER:OG	2.33	0.46
1:A:190:ILE:HD13	1:A:384:ILE:HD13	1.97	0.46
1:A:220:VAL:CG2	1:A:336:THR:HG23	2.44	0.46
1:A:496:VAL:HG21	1:A:506:ILE:HD13	1.98	0.46
2:C:231:THR:HG22	2:C:232:ARG:N	2.31	0.46
2:C:389:MET:HE2	2:C:391:LEU:HD21	1.98	0.46
1:A:365:MET:C	1:A:366:VAL:HG23	2.40	0.46
1:A:396:PHE:CE2	1:A:444:PRO:HD2	2.51	0.46
1:B:689:TYR:CD2	1:B:737:LEU:HD22	2.50	0.46
2:D:63:ASP:HA	2:D:249:HIS:ND1	2.30	0.46
1:A:565:TYR:CA	1:A:568:THR:OG1	2.63	0.46
1:A:709:LEU:N	1:A:710:PRO:CD	2.79	0.46
1:B:239:THR:HB	1:B:242:ASP:OD1	2.16	0.46
1:B:474:LEU:HD12	1:B:474:LEU:C	2.40	0.46
2:C:366:ILE:HD12	2:C:366:ILE:N	2.31	0.46
1:B:173:PHE:HA	1:B:176:PHE:CD2	2.50	0.45
1:B:490:GLY:HA3	1:B:559:GLU:HB2	1.97	0.45
2:C:612:VAL:HB	2:C:614:ASP:OD2	2.16	0.45
1:A:239:THR:HG22	1:A:241:LYS:H	1.81	0.45
1:A:483:ASN:ND2	1:A:540:ALA:HB3	2.32	0.45
1:B:186:HIS:CE1	1:B:316:PHE:CZ	3.04	0.45
2:C:391:LEU:HD12	2:C:588:VAL:CG2	2.46	0.45
2:D:392:ASP:O	2:D:396:VAL:HG23	2.16	0.45
1:A:202:ILE:HB	1:A:210:VAL:HG11	1.98	0.45
1:A:307:ASP:OD1	1:A:307:ASP:C	2.59	0.45
1:A:500:PRO:HB3	1:A:613:ARG:CG	2.47	0.45
1:A:588:ARG:HG2	1:A:588:ARG:HH11	1.80	0.45
1:B:234:HIS:CE1	1:B:236:ASN:HA	2.51	0.45
1:B:545:LEU:HD11	1:B:682:GLU:OE1	2.16	0.45
1:A:214:GLU:HG2	1:A:215:ASN:N	2.31	0.45
1:A:250:VAL:O	1:A:250:VAL:CG1	2.64	0.45
1:B:279:VAL:HB	1:B:334:VAL:HG22	1.99	0.45
1:B:402:TYR:HB3	1:B:447:SER:HB2	1.98	0.45
2:D:316:GLY:O	2:D:320:VAL:HG23	2.16	0.45
1:A:618:LEU:CD2	1:A:701:PHE:HZ	2.30	0.45
1:B:232:LEU:HB2	1:B:373:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:THR:O	1:B:322:PRO:HD3	2.17	0.45
2:C:30:ILE:HG22	2:C:31:PRO:N	2.32	0.45
2:C:421:THR:HA	2:C:422:PRO:HD3	1.84	0.45
1:A:434:SER:O	1:A:438:LEU:HD23	2.16	0.45
1:A:501:LEU:HD23	1:A:611:TYR:HA	1.98	0.45
1:A:686:LEU:HA	1:A:699:HIS:HA	1.98	0.45
1:B:474:LEU:CD1	1:B:550:ILE:HD11	2.46	0.45
1:B:543:PRO:O	1:B:547:TYR:HB3	2.16	0.45
1:A:396:PHE:CD2	1:A:444:PRO:HD2	2.51	0.45
1:B:479:PHE:CE1	1:B:601:LEU:HB3	2.47	0.45
1:A:295:LEU:CD2	1:A:570:MET:HG3	2.47	0.45
1:A:705:GLY:O	1:A:711:ALA:HB2	2.17	0.45
2:D:671:LEU:HD13	2:D:671:LEU:O	2.17	0.45
1:A:319:THR:O	1:A:322:PRO:HD3	2.17	0.45
1:A:588:ARG:HG2	1:A:588:ARG:NH1	2.32	0.45
1:A:712:LEU:HD23	1:A:712:LEU:C	2.42	0.45
2:D:151:ALA:HB1	2:D:169:GLN:HB2	1.99	0.45
2:D:383:ASN:ND2	2:D:384:GLY:N	2.65	0.45
1:A:295:LEU:HD22	1:A:570:MET:HG3	1.98	0.45
1:A:406:GLY:HA2	1:A:451:ALA:O	2.16	0.45
1:B:210:VAL:CG1	1:B:211:TYR:H	2.28	0.45
1:B:389:ILE:N	1:B:389:ILE:HD12	2.32	0.45
2:C:52:ILE:HG22	2:C:254:ARG:HG3	1.98	0.45
2:C:186:PHE:H	2:C:190:GLY:HA3	1.81	0.45
1:A:202:ILE:HG12	1:A:373:VAL:HG12	1.98	0.44
1:A:537:LEU:HD12	1:A:537:LEU:N	2.32	0.44
1:B:182:TRP:HZ3	1:B:392:VAL:HG12	1.82	0.44
2:C:34:GLY:H	2:C:35:PRO:HD2	1.81	0.44
2:C:80:VAL:O	2:C:305:VAL:HB	2.17	0.44
2:C:121:GLY:HA2	2:C:160:PRO:HD2	1.99	0.44
2:D:382:MET:HE3	2:D:402:CYS:HB3	1.99	0.44
2:D:645:ASN:HB3	2:D:650:TYR:HB2	1.98	0.44
1:A:575:GLU:O	1:A:579:ARG:HG3	2.17	0.44
2:C:400:GLY:HA3	2:C:647:TYR:HB3	1.99	0.44
1:A:436:MET:O	1:A:442:PHE:HB3	2.18	0.44
2:C:85:TYR:HE2	2:C:248:SER:HB2	1.83	0.44
2:C:408:LEU:HB2	2:C:587:VAL:HB	1.99	0.44
1:A:460:SER:OG	1:A:540:ALA:HA	2.17	0.44
1:B:523:TYR:OH	1:B:526:SER:HA	2.18	0.44
2:C:274:PHE:O	2:C:284:LEU:N	2.51	0.44
1:B:146:LEU:HD23	1:B:146:LEU:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:TYR:HB2	1:B:571:ASP:HB2	1.99	0.44
2:C:11:VAL:O	2:C:15:GLU:HB3	2.17	0.44
2:C:173:LEU:HD23	2:C:194:CYS:SG	2.57	0.44
1:A:291:VAL:HA	1:B:524:GLN:O	2.17	0.44
1:A:515:HIS:ND1	1:A:516:PRO:HD2	2.32	0.44
2:C:95:TYR:HE1	2:C:247:PRO:O	2.00	0.44
2:C:185:TYR:CD1	2:C:194:CYS:HB2	2.53	0.44
1:A:165:LEU:O	1:A:169:VAL:HG23	2.18	0.44
2:C:144:LYS:HA	2:C:145:PRO:C	2.41	0.44
1:A:127:LEU:CD2	1:A:442:PHE:CD1	3.01	0.44
1:A:254:ILE:HD12	1:A:373:VAL:HG23	2.00	0.44
1:A:426:LEU:HD11	1:A:450:PHE:HB3	2.00	0.44
1:B:131:LEU:HD22	1:B:599:ILE:CD1	2.48	0.44
1:A:295:LEU:CD2	1:A:568:THR:HG21	2.48	0.43
1:A:453:TRP:CE3	1:A:463:ALA:HA	2.52	0.43
1:A:651:ARG:HH22	2:C:356:ASP:CG	2.26	0.43
1:B:243:PHE:HA	1:B:246:LEU:HD12	1.99	0.43
2:C:643:ASP:O	2:C:645:ASN:N	2.50	0.43
2:D:381:ILE:HD11	2:D:389:MET:HG2	2.00	0.43
1:A:264:PHE:HD1	1:A:281:ILE:HD13	1.83	0.43
1:A:298:PHE:CG	1:A:299:GLY:N	2.86	0.43
1:B:448:ILE:HD13	1:B:598:VAL:HG11	2.00	0.43
2:C:676:PHE:CD1	2:C:677:ARG:HG3	2.53	0.43
2:D:350:HIS:HB2	2:D:629:LEU:HD21	1.99	0.43
2:D:374:THR:O	2:D:378:ILE:HG13	2.19	0.43
2:D:612:VAL:O	2:D:614:ASP:N	2.48	0.43
2:C:158:CYS:HB2	2:C:173:LEU:HB2	1.99	0.43
2:D:5:THR:HA	2:D:36:SER:HB3	2.00	0.43
1:A:263:THR:HG1	1:A:266:GLU:CG	2.29	0.43
1:B:559:GLU:HG3	1:B:560:ASP:N	2.34	0.43
1:A:134:LYS:NZ	1:A:435:ASP:HB3	2.34	0.43
1:B:470:TYR:CD1	1:B:470:TYR:N	2.86	0.43
1:B:498:ALA:CB	1:B:553:VAL:HA	2.48	0.43
2:C:225:LEU:HD13	2:C:235:VAL:HG13	2.01	0.43
2:C:352:ARG:HG3	2:C:353:LEU:N	2.33	0.43
1:A:258:ARG:HG2	1:A:282:TYR:CZ	2.53	0.43
1:B:129:ARG:O	1:B:133:GLU:HG3	2.19	0.43
1:B:182:TRP:CE2	1:B:390:PHE:HB2	2.52	0.43
1:B:682:GLU:OE1	1:B:699:HIS:NE2	2.46	0.43
2:C:615:CYS:O	2:C:618:ASN:O	2.36	0.43
1:A:276:ALA:O	1:A:332:ILE:HD11	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLY:C	1:B:461:VAL:HG22	2.43	0.43
2:C:62:LEU:HD23	2:C:252:VAL:CG2	2.47	0.43
2:C:80:VAL:HG23	2:C:81:VAL:N	2.34	0.43
2:D:130:ILE:H	2:D:131:PRO:HD2	1.84	0.43
2:D:407:VAL:CG1	2:D:594:GLU:HG3	2.48	0.43
1:A:625:LEU:HB2	1:A:713:LEU:HD21	2.00	0.43
1:B:353:CYS:HA	1:B:354:PRO:HD3	1.92	0.43
2:D:671:LEU:HD13	2:D:671:LEU:C	2.44	0.43
1:A:155:ARG:CD	1:A:409:ARG:O	2.63	0.43
2:C:61:THR:HA	2:C:251:VAL:HA	2.00	0.43
2:C:84:PHE:CZ	2:C:301:GLY:HA3	2.54	0.43
1:A:220:VAL:HA	1:A:299:GLY:O	2.19	0.42
1:A:501:LEU:CD2	1:A:611:TYR:HA	2.49	0.42
1:B:500:PRO:HB3	1:B:613:ARG:HG3	2.00	0.42
1:A:224:LYS:O	1:A:224:LYS:HG2	2.20	0.42
1:B:212:LEU:C	1:B:212:LEU:HD23	2.45	0.42
1:B:446:ARG:NE	1:B:607:LEU:HD21	2.34	0.42
1:A:306:GLY:C	1:A:461:VAL:HG22	2.44	0.42
2:C:363:VAL:HG12	2:C:363:VAL:O	2.19	0.42
1:A:366:VAL:CG1	1:A:367:THR:N	2.83	0.42
1:A:677:ARG:NH2	1:A:750:SER:O	2.53	0.42
1:B:513:VAL:HB	1:B:522:LEU:HD12	2.00	0.42
1:B:689:TYR:OH	1:B:740:TRP:HD1	2.01	0.42
1:B:700:VAL:HB	1:B:709:LEU:HD13	2.00	0.42
2:C:259:LYS:O	2:C:259:LYS:HG3	2.19	0.42
1:A:448:ILE:HD13	1:A:598:VAL:CG1	2.49	0.42
1:B:186:HIS:CE1	1:B:465:GLU:HB3	2.54	0.42
1:B:433:PHE:O	1:B:437:VAL:HG23	2.19	0.42
2:D:48:CYS:O	2:D:51:ALA:HB3	2.20	0.42
2:D:81:VAL:HB	2:D:251:VAL:HB	2.01	0.42
1:A:392:VAL:HG23	1:A:449:ILE:HG12	2.02	0.42
1:A:496:VAL:HG13	1:A:496:VAL:O	2.19	0.42
1:A:607:LEU:C	1:A:609:LEU:H	2.27	0.42
1:B:232:LEU:HA	1:B:254:ILE:O	2.20	0.42
2:C:26:MET:O	2:C:30:ILE:HG12	2.19	0.42
2:C:105:SER:H	2:C:232:ARG:HH12	1.67	0.42
2:D:119:HIS:HB2	2:D:159:ALA:HA	2.02	0.42
1:A:563:TYR:HA	1:A:564:PRO:HD3	1.89	0.42
2:C:45:TYR:CD2	2:C:66:LEU:HD13	2.54	0.42
1:A:179:SER:OG	1:A:393:ILE:HA	2.19	0.42
1:A:490:GLY:HA3	1:A:559:GLU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:PHE:O	1:A:601:LEU:HD12	2.19	0.42
1:A:749:LEU:O	1:A:750:SER:C	2.63	0.42
2:D:144:LYS:HA	2:D:145:PRO:C	2.44	0.42
2:D:380:LYS:O	2:D:383:ASN:ND2	2.53	0.42
1:A:576:LEU:CD1	1:A:580:ILE:HD12	2.49	0.41
1:A:756:ILE:O	1:A:756:ILE:CG1	2.66	0.41
1:B:604:ASP:OD2	1:B:606:GLU:HB2	2.20	0.41
2:D:70:ALA:HB1	2:D:77:LEU:HB2	2.01	0.41
1:A:365:MET:C	1:A:366:VAL:CG2	2.93	0.41
2:C:19:CYS:O	2:C:22:PHE:HB3	2.20	0.41
2:C:45:TYR:CZ	2:C:66:LEU:HD22	2.55	0.41
2:C:665:CYS:SG	2:C:666:SER:N	2.93	0.41
1:A:329:LEU:HA	1:A:330:PRO:HD3	1.88	0.41
1:B:464:THR:O	1:B:468:GLU:HG3	2.21	0.41
2:D:602:ARG:O	2:D:605:GLN:HB2	2.20	0.41
2:D:605:GLN:HE21	2:D:605:GLN:HB3	1.57	0.41
1:A:692:PRO:O	1:A:696:PRO:HA	2.20	0.41
1:B:367:THR:HG22	1:B:368:SER:H	1.85	0.41
1:B:542:PHE:N	1:B:543:PRO:CD	2.83	0.41
2:C:365:LYS:C	2:C:366:ILE:HD12	2.45	0.41
2:C:626:THR:OG1	2:C:629:LEU:HD11	2.20	0.41
2:D:632:ARG:CB	2:D:635:THR:OG1	2.64	0.41
1:A:349:MET:HG2	1:A:367:THR:HG22	2.02	0.41
1:A:480:THR:CG2	1:A:481:TYR:N	2.83	0.41
1:A:182:TRP:CZ3	1:A:392:VAL:HB	2.55	0.41
1:A:295:LEU:HD22	1:A:570:MET:SD	2.60	0.41
1:B:444:PRO:HB2	1:B:602:THR:CG2	2.51	0.41
1:B:568:THR:OG1	1:B:570:MET:CG	2.68	0.41
1:B:568:THR:CB	1:B:570:MET:HG2	2.51	0.41
1:B:718:LEU:HB2	1:B:726:PHE:HB2	2.01	0.41
1:A:193:LYS:CD	1:A:219:TYR:HB3	2.43	0.41
1:B:448:ILE:HD13	1:B:598:VAL:CG1	2.51	0.41
1:B:719:ARG:HD3	1:B:726:PHE:CE2	2.55	0.41
2:D:306:PRO:HA	2:D:307:PRO:HD3	1.92	0.41
1:B:252:GLY:HA2	1:B:277:ILE:HD11	2.02	0.41
1:B:397:VAL:HG12	1:B:398:GLU:HG3	2.03	0.41
1:A:236:ASN:CG	1:A:237:PHE:N	2.79	0.41
1:A:305:THR:HG23	1:A:697:PHE:CZ	2.56	0.41
1:A:700:VAL:HB	1:A:709:LEU:CD1	2.51	0.41
1:B:236:ASN:CG	1:B:237:PHE:H	2.27	0.41
1:B:446:ARG:NH1	1:B:446:ARG:HG3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:TYR:HB3	1:B:473:SER:HB3	2.02	0.41
1:B:537:LEU:HD12	1:B:537:LEU:N	2.36	0.41
2:D:145:PRO:HG2	2:D:148:LYS:CB	2.51	0.41
2:D:326:LEU:HD23	2:D:326:LEU:C	2.46	0.41
1:A:565:TYR:CD2	1:A:570:MET:CB	3.04	0.40
1:B:703:GLY:O	1:B:708:THR:HG21	2.21	0.40
1:B:740:TRP:CE3	1:B:740:TRP:HA	2.57	0.40
2:C:30:ILE:HA	2:C:31:PRO:HA	1.81	0.40
1:A:310:THR:N	1:A:311:PRO:CD	2.85	0.40
1:A:459:GLY:C	1:A:461:VAL:N	2.78	0.40
1:A:498:ALA:CB	1:A:553:VAL:HA	2.50	0.40
1:A:565:TYR:CG	1:A:570:MET:HB3	2.57	0.40
1:B:228:VAL:HB	1:B:277:ILE:HG22	2.03	0.40
1:B:412:TRP:HH2	1:B:569:THR:HG23	1.71	0.40
1:A:193:LYS:HG3	1:A:219:TYR:CG	2.57	0.40
1:A:305:THR:HG1	1:A:697:PHE:HE1	1.63	0.40
1:A:680:ARG:O	1:A:682:GLU:N	2.55	0.40
1:B:709:LEU:N	1:B:710:PRO:CD	2.84	0.40
2:C:319:TYR:CE2	2:C:323:ILE:HD11	2.56	0.40
2:D:406:PRO:HA	2:D:588:VAL:HA	2.02	0.40
1:A:234:HIS:CE1	1:A:236:ASN:HA	2.57	0.40
1:A:353:CYS:HA	1:A:354:PRO:HD3	1.93	0.40
1:A:493:ASN:ND2	1:A:495:LYS:HE3	2.34	0.40
1:A:565:TYR:HE1	1:A:579:ARG:HD2	1.85	0.40
1:B:132:SER:HA	1:B:135:LEU:HD12	2.04	0.40
2:C:121:GLY:HA2	2:C:160:PRO:HB2	2.03	0.40
2:C:349:HIS:O	2:C:352:ARG:HG2	2.21	0.40
1:A:474:LEU:C	1:A:474:LEU:HD12	2.47	0.40
1:B:402:TYR:CE1	1:B:478:ALA:HB2	2.56	0.40
1:B:500:PRO:O	1:B:613:ARG:HG2	2.22	0.40
2:D:317:TYR:CD2	2:D:590:ARG:HD2	2.56	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	636/654 (97%)	588 (92%)	43 (7%)	5 (1%)	16	48
1	B	637/654 (97%)	603 (95%)	32 (5%)	2 (0%)	36	67
2	C	509/693 (73%)	464 (91%)	39 (8%)	6 (1%)	10	40
2	D	467/693 (67%)	434 (93%)	29 (6%)	4 (1%)	14	46
All	All	2249/2694 (84%)	2089 (93%)	143 (6%)	17 (1%)	16	48

All (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
2	C	34	GLY
1	A	154	PRO
1	B	210	VAL
2	C	76	ASN
2	D	76	ASN
1	A	475	HIS
2	C	628	ASP
2	D	339	CYS
1	A	750	SER
1	B	190	ILE
2	C	306	PRO
2	C	31	PRO

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%)	514 (99%)	7 (1%)	61	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	483/562 (86%)	479 (99%)	4 (1%)	73	80
2	C	353/585 (60%)	350 (99%)	3 (1%)	73	80
2	D	291/585 (50%)	290 (100%)	1 (0%)	86	87
All	All	1648/2294 (72%)	1633 (99%)	15 (1%)	70	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
1	A	297	PHE
1	A	320	GLN
1	A	357	TRP
1	A	511	GLN
1	A	565	TYR
1	A	753	VAL
1	B	197	GLN
1	B	251	ASN
1	B	320	GLN
1	B	603	HIS
2	C	129	ASN
2	C	241	CYS
2	C	377	CYS
2	D	383	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	160	GLN
1	A	164	ASN
1	A	172	GLN
1	A	185	GLN
1	A	275	ASN
1	A	285	GLN
1	A	335	GLN
1	A	431	GLN
1	A	493	ASN
1	A	511	GLN
1	A	524	GLN
1	A	627	GLN

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Mol	Chain	Res	Type
1	A	743	GLN
1	A	747	ASN
1	A	758	ASN
1	B	160	GLN
1	B	236	ASN
1	B	285	GLN
1	B	292	ASN
1	B	335	GLN
1	B	483	ASN
1	B	512	ASN
1	B	524	GLN
1	B	596	GLN
1	B	627	GLN
1	B	715	ASN
1	B	734	GLN
1	B	743	GLN
1	B	747	ASN
2	C	129	ASN
2	C	207	HIS
2	C	271	GLN
2	C	584	ASN
2	C	585	HIS
2	C	603	GLN
2	C	604	GLN
2	C	661	ASN
2	D	14	HIS
2	D	111	GLN
2	D	129	ASN
2	D	325	ASN
2	D	383	ASN
2	D	411	ASN
2	D	584	ASN
2	D	603	GLN
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	$\# Z > 2$
6	CO3	D	905	5	3,3,3	0.23	0	2,3,3	0.13	0
3	NAG	A	903	1	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
3	NAG	B	903	1	14,14,15	0.44	0	17,19,21	1.16	2 (11%)
6	CO3	C	905	5	3,3,3	0.29	0	2,3,3	0.26	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	A	903	1	-	0/6/23/26	0/1/1/1
3	NAG	B	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(°)	Ideal(°)
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 [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	638/654 (97%)	0.18	29 (4%) 38 24	45, 81, 127, 200	0
1	B	639/654 (97%)	0.77	81 (12%) 8 6	39, 106, 184, 200	1 (0%)
2	C	515/693 (74%)	0.91	65 (12%) 8 6	70, 127, 182, 200	2 (0%)
2	D	487/693 (70%)	0.78	45 (9%) 14 10	68, 150, 199, 200	1 (0%)
All	All	2279/2694 (84%)	0.64	220 (9%) 13 9	39, 111, 185, 200	4 (0%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	752	ASP	6.4
2	C	189	SER	5.2
1	B	235	ALA	5.0
1	B	264	PHE	5.0
2	D	631	PHE	4.8
2	C	301	GLY	4.6
2	C	270	ALA	4.5
1	B	154	PRO	4.4
1	B	753	VAL	4.2
1	B	417	ALA	4.2
2	C	269	GLN	4.1
1	A	211	TYR	4.0
1	A	752	ASP	4.0
2	C	97	ALA	4.0
2	C	210	ILE	3.9
2	C	224	GLU	3.8
2	D	205	VAL	3.8
1	A	264	PHE	3.8
2	D	630	LEU	3.8
1	B	215	ASN	3.7
2	D	189	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	759	GLU	3.7
1	A	751	GLY	3.7
1	B	751	GLY	3.7
1	A	750	SER	3.7
1	B	201	ILE	3.7
1	B	396	PHE	3.7
1	A	261	LYS	3.6
1	A	194	ASP	3.6
1	B	155	ARG	3.6
2	D	425	GLY	3.6
2	C	39	CYS	3.5
1	B	298	PHE	3.5
1	B	380	VAL	3.4
2	C	25	HIS	3.4
1	B	373	VAL	3.4
2	D	629	LEU	3.3
2	D	583	PRO	3.3
1	B	250	VAL	3.3
2	D	71	TYR	3.3
1	B	217	GLY	3.3
2	C	284	LEU	3.2
2	C	6	VAL	3.2
2	D	128	TRP	3.2
2	C	53	ALA	3.2
1	B	565	TYR	3.2
1	B	517	VAL	3.2
1	A	305	THR	3.2
2	C	665	CYS	3.2
1	B	640	GLN	3.2
2	D	393	GLY	3.2
2	C	295	PHE	3.2
1	B	157	ALA	3.1
1	B	336	THR	3.1
1	B	570	MET	3.1
1	A	260	GLY	3.1
1	B	200	VAL	3.0
2	C	302	PHE	3.0
2	C	613	THR	3.0
2	D	168	PRO	3.0
1	B	324	SER	3.0
1	B	233	VAL	2.9
1	B	212	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	185	TYR	2.9
1	B	569	THR	2.9
2	C	204	PHE	2.9
1	A	197	GLN	2.9
2	D	424	ALA	2.9
1	B	563	TYR	2.9
1	B	331	ASN	2.9
1	A	706	SER	2.8
1	B	214	GLU	2.8
2	D	181	THR	2.8
1	B	337	ILE	2.8
2	D	85	TYR	2.8
1	A	195	SER	2.8
2	D	131	PRO	2.8
2	C	647	TYR	2.8
2	D	252	VAL	2.8
1	B	379	ASN	2.7
1	A	636	GLY	2.7
2	C	275	GLY	2.7
2	D	613	THR	2.7
1	B	282	TYR	2.7
2	D	611	ASP	2.7
1	B	422	GLY	2.6
1	B	199	SER	2.6
1	B	203	VAL	2.6
2	D	169	GLN	2.6
2	D	206	LYS	2.6
2	C	5	THR	2.6
1	A	196	ALA	2.6
2	D	336	THR	2.6
2	C	28	SER	2.6
1	B	153	VAL	2.6
2	C	68	TYR	2.6
1	A	704	SER	2.6
2	C	12	SER	2.6
2	D	397	TYR	2.5
1	A	399	PRO	2.5
2	C	36	SER	2.5
2	C	62	LEU	2.5
1	B	613	ARG	2.5
2	C	30	ILE	2.5
2	D	234	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	432	MET	2.5
2	C	71	TYR	2.5
2	D	294	LEU	2.5
2	C	610	SER	2.5
1	B	202	ILE	2.5
1	B	727	ASN	2.5
2	C	636	VAL	2.5
1	A	259	ALA	2.5
2	D	81	VAL	2.5
2	C	21	SER	2.4
2	D	267	LEU	2.4
2	C	172	GLN	2.4
1	B	254	ILE	2.4
2	C	271	GLN	2.4
1	B	146	LEU	2.4
2	C	31	PRO	2.4
1	B	347	GLY	2.4
1	B	187	PHE	2.4
1	B	192	VAL	2.4
1	B	210	VAL	2.4
1	B	306	GLY	2.3
2	D	659	VAL	2.3
2	D	647	TYR	2.3
1	A	749	LEU	2.3
2	D	94	PHE	2.3
2	C	126	ALA	2.3
2	C	249	HIS	2.3
2	C	273	HIS	2.3
1	B	758	ASN	2.3
2	C	24	ASP	2.3
1	A	754	TRP	2.3
1	B	296	SER	2.3
2	C	646	THR	2.3
2	D	120	THR	2.3
2	C	606	HIS	2.3
1	A	396	PHE	2.3
1	B	297	PHE	2.3
1	B	160	GLN	2.3
2	C	609	GLY	2.3
1	B	412	TRP	2.3
1	A	720	LYS	2.3
2	C	644	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	423	GLU	2.2
2	C	26	MET	2.2
2	C	49	ILE	2.2
1	B	636	GLY	2.2
2	C	10	ALA	2.2
2	C	206	LYS	2.2
2	C	188	TYR	2.2
1	B	488	VAL	2.2
2	C	15	GLU	2.2
1	B	571	ASP	2.2
2	D	97	ALA	2.2
2	D	8	TRP	2.2
1	A	689	TYR	2.2
1	B	348	ASN	2.2
2	C	293	LEU	2.2
1	B	391	GLY	2.2
1	B	414	PRO	2.2
2	D	82	ALA	2.2
1	B	384	ILE	2.2
2	D	157	SER	2.2
1	B	381	LEU	2.2
2	C	59	ALA	2.2
1	B	278	GLY	2.2
2	C	113	ARG	2.2
2	D	132	ILE	2.1
1	B	387	LEU	2.1
2	C	180	SER	2.1
2	D	208	SER	2.1
1	B	458	PHE	2.1
1	A	757	ASP	2.1
2	D	349	HIS	2.1
1	B	566	LEU	2.1
1	B	365	MET	2.1
1	B	225	ALA	2.1
1	B	579	ARG	2.1
1	A	314	PRO	2.1
1	B	260	GLY	2.1
2	D	36	SER	2.1
2	C	282	PHE	2.1
2	C	622	PHE	2.1
1	A	373	VAL	2.1
2	C	367	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	79	PRO	2.1
2	D	282	PHE	2.1
2	C	213	ASN	2.1
2	C	264	TRP	2.1
2	D	108	GLN	2.1
1	B	415	GLY	2.1
2	C	81	VAL	2.1
2	C	363	VAL	2.1
2	D	67	VAL	2.1
1	B	150	ASN	2.1
2	C	300	HIS	2.1
2	D	207	HIS	2.1
2	D	643	ASP	2.1
1	A	568	THR	2.1
1	B	222	TYR	2.1
1	B	309	TYR	2.1
2	C	281	GLU	2.1
1	A	153	VAL	2.0
1	B	141	THR	2.0
1	B	226	ALA	2.0
2	C	292	ASP	2.0
2	D	292	ASP	2.0
1	A	721	GLN	2.0
1	B	416	ALA	2.0
1	B	219	TYR	2.0
1	B	299	GLY	2.0
1	B	490	GLY	2.0
2	C	114	GLY	2.0
2	C	211	PHE	2.0
1	B	258	ARG	2.0
1	A	209	LEU	2.0

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 oligosaccharides 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	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	0.04	98,98,98,98	0
4	CA	B	900	1/1	0.98	0.03	79,79,79,79	0
4	CA	A	900	1/1	0.99	0.07	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.