Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 07:53 AM BST

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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

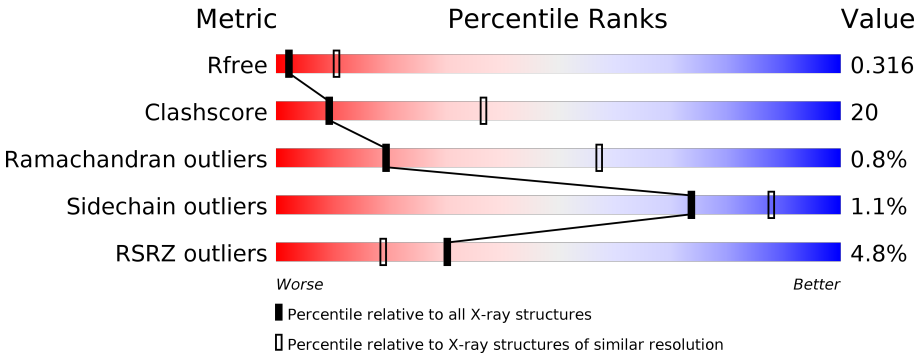
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 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}	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (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 on 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	59% 37%
1	B	654	4% 65% 32%
2	C	693	3% 55% 19% 26%
2	D	693	7% 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CO3	D	905	-	-	X	-

2 Entry composition (i)

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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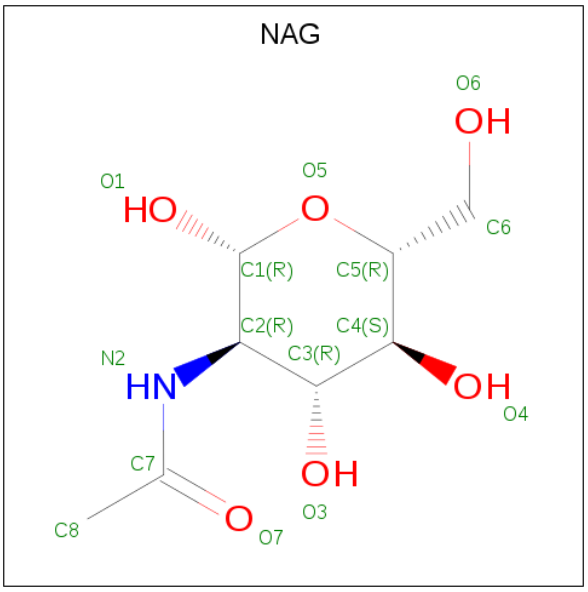
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP P02787
D	-4	HIS	-	expression tag	UNP P02787
D	-3	ILE	-	expression tag	UNP P02787
D	-2	GLU	-	expression tag	UNP P02787
D	-1	GLY	-	expression tag	UNP P02787
D	0	ARG	-	expression tag	UNP P02787
D	413	ASP	ASN	engineered mutation	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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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

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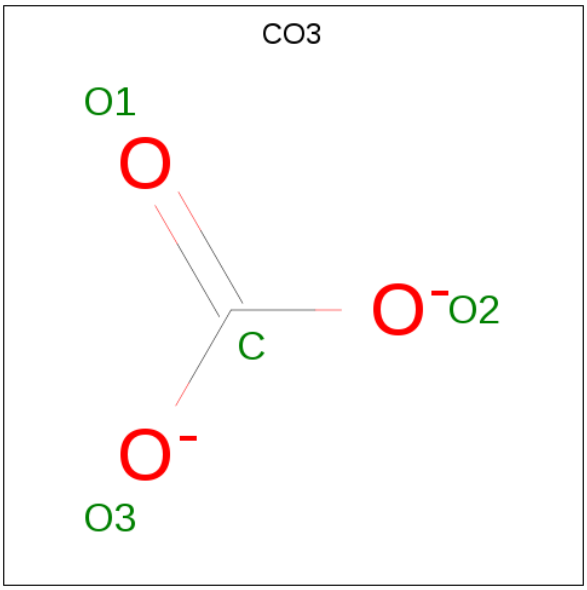
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

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

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

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



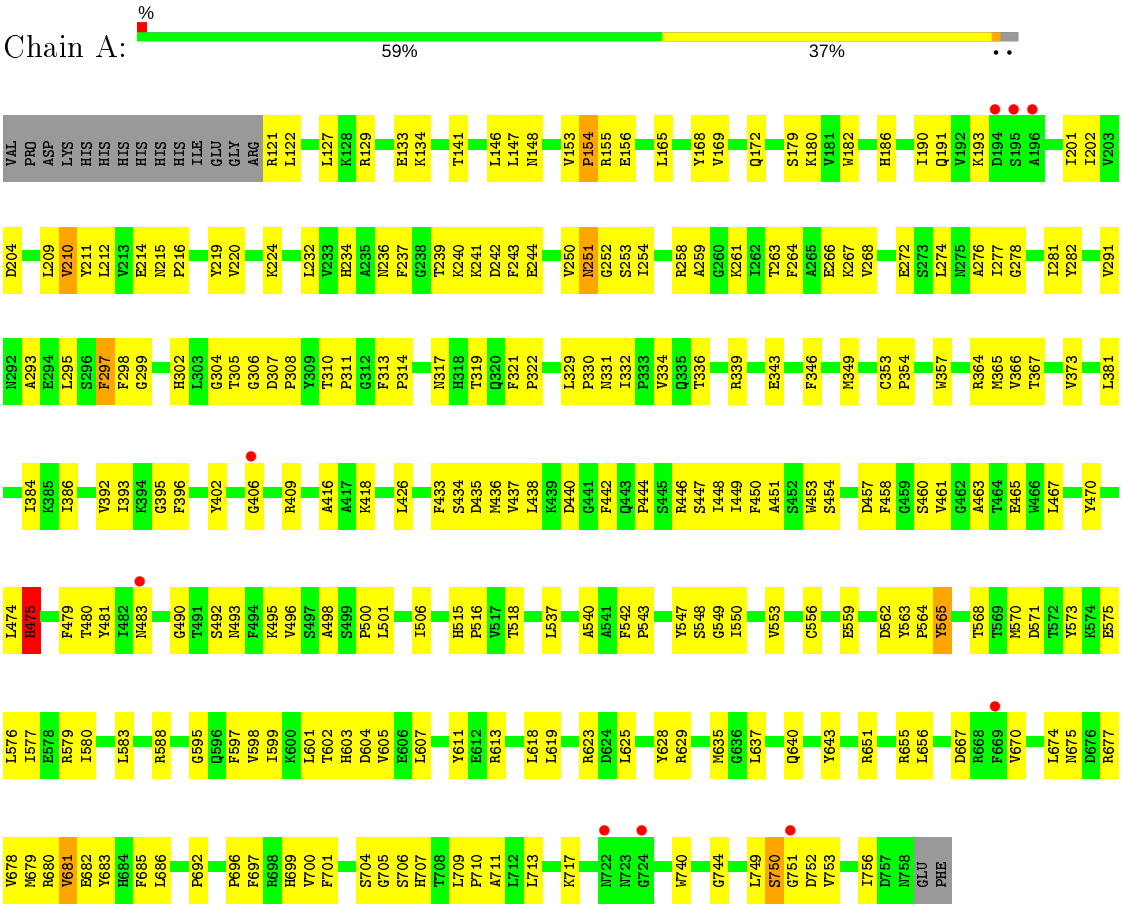
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 1 3	0	0
6	D	1	Total C O 4 1 3	0	0

3 Residue-property plots (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.

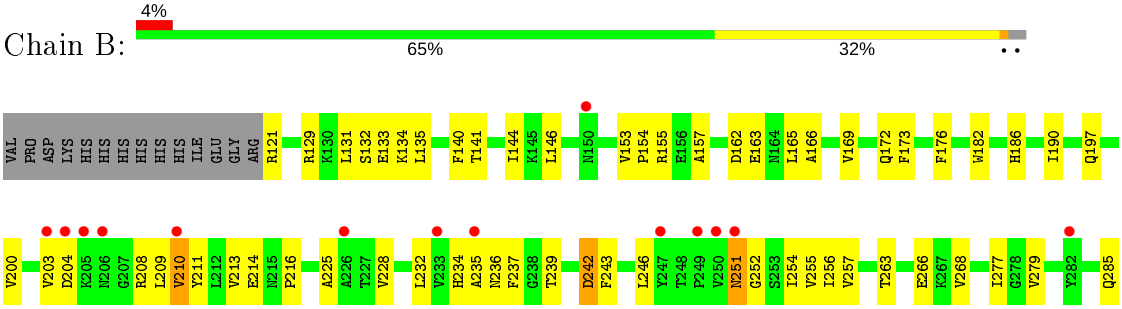
- Molecule 1: Transferrin receptor protein 1

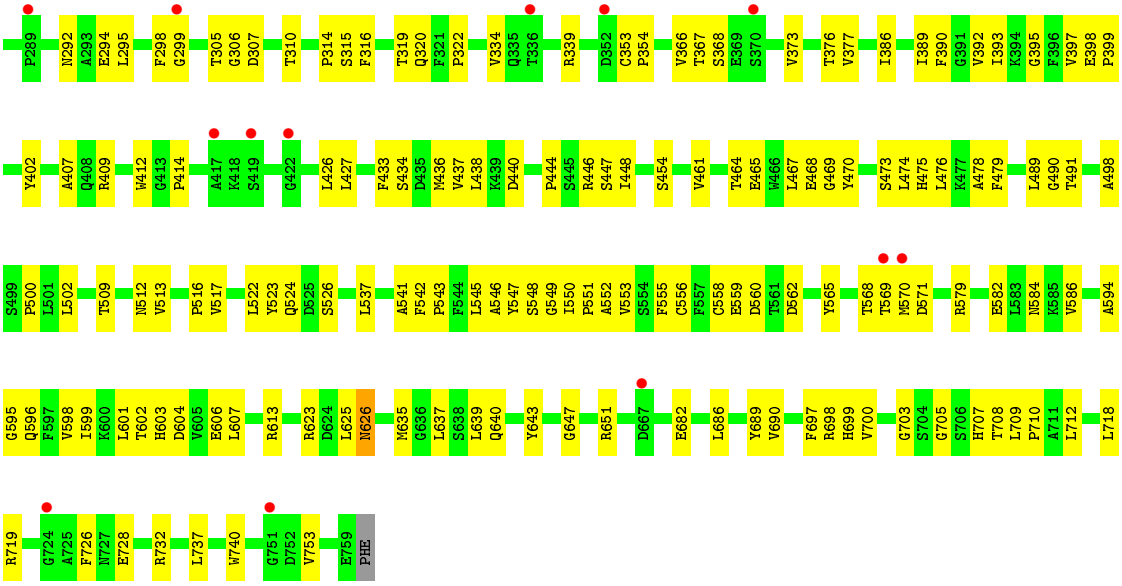
Chain A:



- Molecule 1: Transferrin receptor protein 1

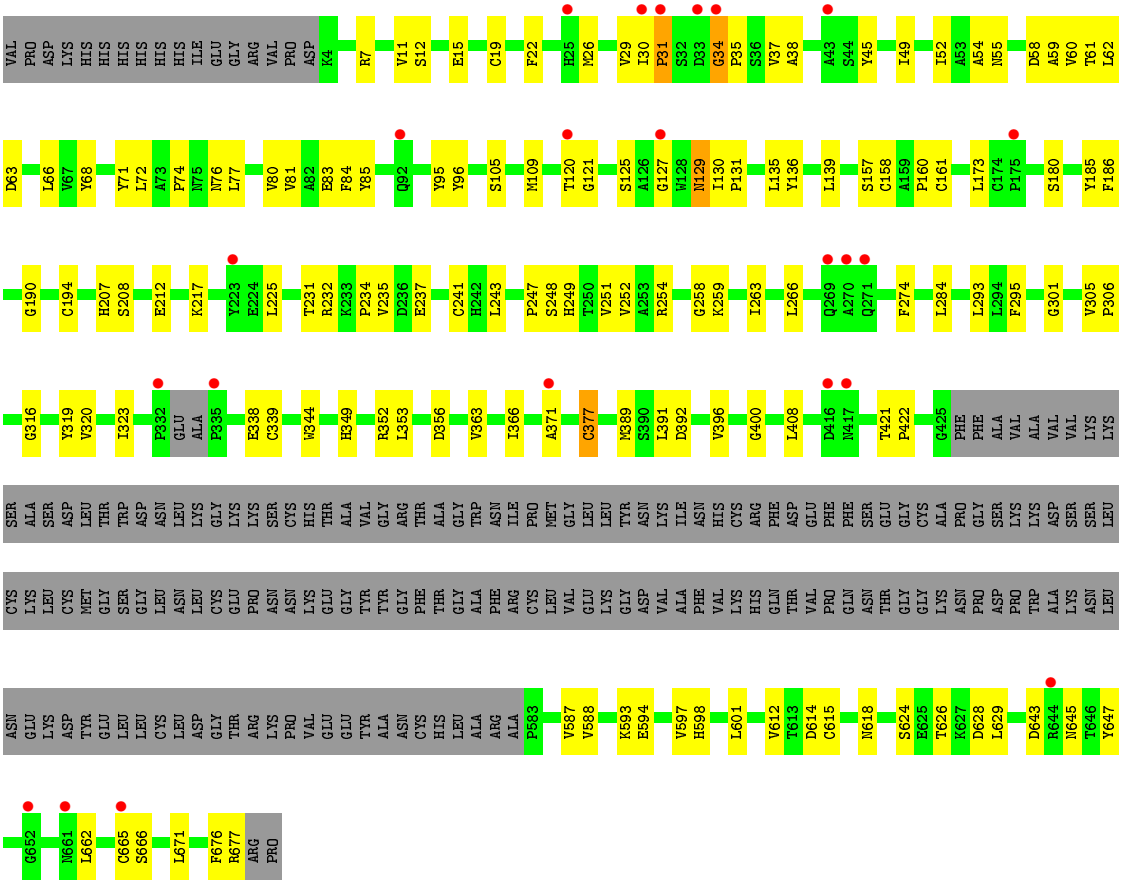
Chain B:





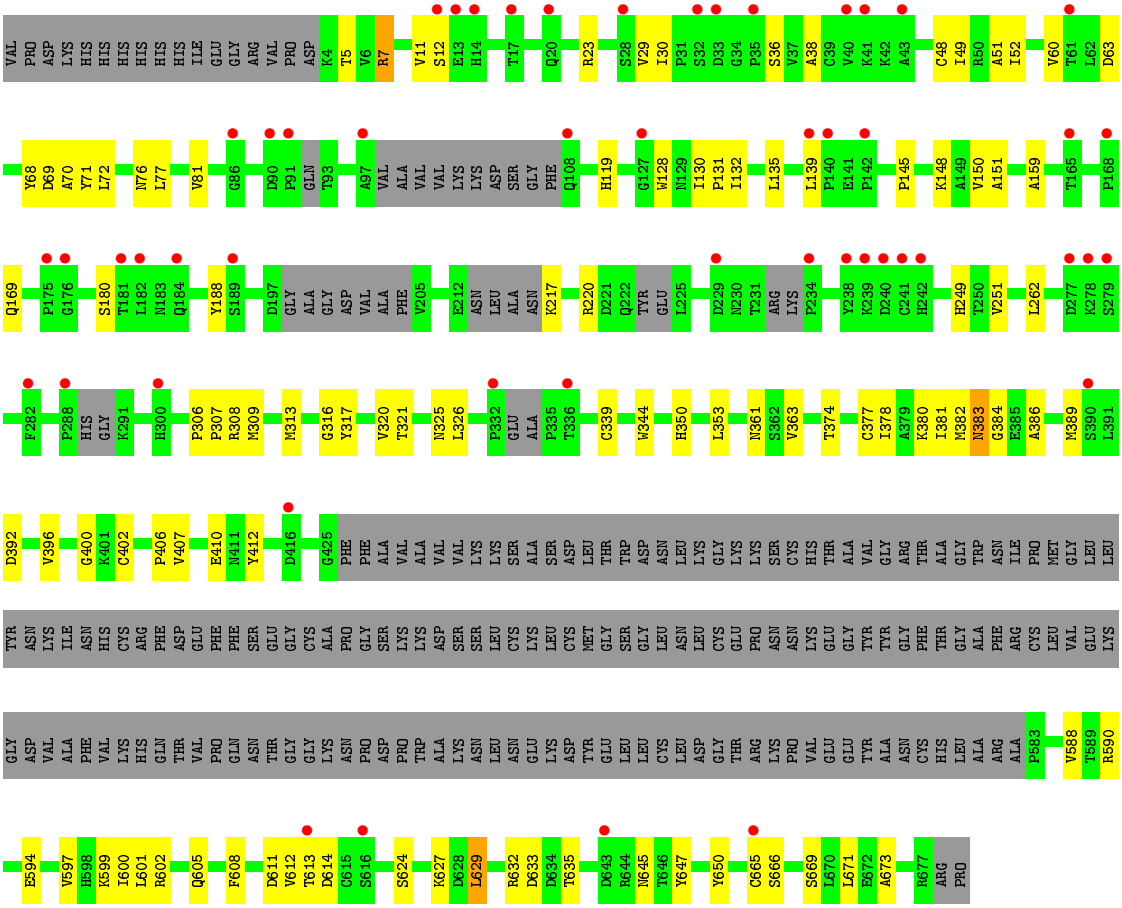
- Molecule 2: Serotransferrin

Chain C:



- Molecule 2: Serotransferrin

Chain D:


VAL PRO ASP LYS HIS HIS HIS HIS HIS HIS ILE GLU GLY ARG VAL PRO ASP K4 T5 V6 R7 V11 S12 E13 H14 T17 Q20 R23 S28 V29 I30 P31 S32 D33 G34 P35 S36 V37 A38 C39 V40 K41 K42 A43 C48 I49 R50 A51 I52 V60 T61 L62 D63
Y68 D69 A70 Y71 L72 N76 L77 V81 G86 D90 P91 GLN T93 A97 VAL ALA VAL VAL LYS LYS ASP SER GLY PHE Q108 H119 G127 W128 N129 I130 P131 I132 L135 L139 P140 E141 P142 P145 K148 A149 V150 A151 A159 T165 P168
Q169 P175 G176 S180 T181 L182 N183 Q184 Y188 S189 D197 GLY ALA GLY ASP VAL ALA PHE V205 E212 ASN LEU ALA ASN K217 R220 D221 Q222 TYR GLU L225 D229 N230 T231 ARG LYS P234 Y238 K239 D240 C241 H242 H249 T250 V251 L262 D277 K278 S279
F282 P288 HIS GLY K291 H300 P306 P307 R308 M309 M313 G316 Y317 V320 T321 N325 L326 P332 GLU ALA P335 T336 C339 W344 H350 L353 N361 S362 V363 T374 C377 I378 A379 K380 I381 M382 N383 G384 E385 A386 M389 S390 L391
D392 V396 G400 K401 C402 P406 V407 E410 N411 Y412 D416 G425 PHE PHE ALA VAL ALA VAL VAL LYS LYS SER ALA SER ASP LEU THR TRP ASP ASN LEU LYS GLY LYS LYS SER CYS HIS THR ALA VAL GLY ARG THR ALA GLY TRP ASN ILE PRO MET GLY LEU LEU
TYR ASN LYS ILE ASN HIS CYS ARG PHE ASP GLU PHE PHE SER GLU GLY CYS ALA PRO GLY SER LYS LYS ASP SER SER LEU CYS LYS LEU CYS MET GLY SER GLY LEU ASN LEU CYS GLU PRO ASN ASN LYS GLU GLY TYR TYR GLY PHE THR GLY ALA PHE ARG CYS LEU VAL GLU LYS
GLY ASP VAL ALA PHE VAL LYS HIS GLN THR VAL PRO GLN ASN THR GLY GLY LYS ASN PRO ASP PRO TRP ALA LYS ASN LEU ASN GLU LYS ASP TYR GLU LEU LEU CYS LEU ASP GLY THR ARG LYS PRO VAL GLU GLU TYR ALA ASN CYS HIS LEU ALA ARG ALA P583 V588 T589 R590
E594 V597 H598 K599 I600 L601 R602 Q605 F608 D611 V612 T613 D614 C615 S616 S624 K627 D628 L629 R632 D633 D634 T635 D643 R644 N645 T646 Y647 Y650 C665 S666 S669 L670 L671 E672 A673 R677 ARG PRO

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 29.94 – 3.22	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.22) 99.5 (29.94-3.22)	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)	0.29 , 85.4	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.*

[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: CO3, FE, CA, NAG

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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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.

All (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
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:677:ARG:NH1	1:A:751:GLY:CA	2.22	1.03
1:A:306:GLY:HA2	1:A:461:VAL:HA	1.04	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:ILE:CG2	2:C:31:PRO:CA	2.50	0.89
2:C:58:ASP:CG	2:C:259:LYS:NZ	2.26	0.88
1:B:153:VAL:CB	1:B:154:PRO:HD3	2.02	0.87
1:A:251:ASN:ND2	1:A:251:ASN:O	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
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
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:A:251:ASN:C	1:A:251:ASN:HD22	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:30:ILE:CG2	2:C:31:PRO:CB	2.67	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:753:VAL:O	1:B:753:VAL:HG12	1.90	0.71
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:HG13	1:A:756:ILE:O	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:626:ASN:HD22	1:B:626:ASN:C	1.95	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
2:D:188:TYR:CE1	6:D:905:CO3:O2	2.48	0.67
2:D:63:ASP:OD1	2:D:249:HIS:CE1	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:251:ASN:HD22	1:B:251:ASN:C	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HD23	2:D:262:LEU:O	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:HB3	1:A:579:ARG:HH11	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
2:D:363:VAL:O	2:D:363:VAL:HG12	2.00	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
1:A:146:LEU:HD23	1:A:146:LEU:O	1.99	0.61
1:B:565:TYR:HB3	1:B:568:THR:HG1	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O	2:C:662:LEU:HD23	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
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:OD2	1:A:562:ASP:N	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
1:A:433:PHE:HE1	1:A:599:ILE:CD1	2.16	0.57
1:B:562:ASP:N	1:B:562:ASP:OD2	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:667:ASP:OD1	2:C:74:PRO:HD3	2.06	0.56
1:A:500:PRO:HB3	1:A:613:ARG:HG3	1.86	0.56
1:A:704:SER:O	1:A:707:HIS:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:CD2	1:A:297:PHE:N	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
1:A:155:ARG:O	1:A:156:GLU:C	2.44	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:HD22	2:D:383:ASN:N	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:62:LEU:HD23	2:C:252:VAL:HG22	1.87	0.55
2:C:29:VAL:O	2:C:29:VAL:HG22	2.07	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:A:680:ARG:O	1:A:681:VAL:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:PHE:HD2	1:A:297:PHE:H	1.54	0.54
1:A:436:MET:HA	1:A:440:ASP:HB2	1.90	0.54
1:A:295:LEU:HD21	1:A:568:THR:CB	2.37	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
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:210:VAL:HG12	1:B:211:TYR:N	2.24	0.53
2:D:23:ARG:HD2	2:D:23:ARG:C	2.29	0.53
1:B:392:VAL:HG22	1:B:393:ILE:N	2.24	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:O	1:B:146:LEU:HD23	2.09	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:A:317:ASN:HA	1:A:321:PHE:CE1	2.45	0.52
1:A:619:LEU:HD23	1:A:619:LEU:O	2.10	0.52
2:D:23:ARG:HD2	2:D:23:ARG:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD2	1:A:297:PHE:N	2.07	0.51
1:B:376:THR:O	1:B:376:THR:HG23	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
2:D:611:ASP:OD1	2:D:612:VAL:N	2.43	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: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:319:TYR:O	2:C:323:ILE:HG13	2.11	0.50
2:C:37:VAL:CG2	2:C:266:LEU:HD21	2.38	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
2:D:632:ARG:HB2	2:D:635:THR:HG1	1.77	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:728:GLU:HG2	1:B:732:ARG:HE	1.77	0.50
1:A:579:ARG:CB	1:A:579:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:382:MET:CE	2:D:402:CYS:HB3	2.42	0.49
1:A:224:LYS:HD2	1:A:331:ASN:C	2.33	0.49
1:B:516:PRO:HG3	1:B:586:VAL:HA	1.95	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:NH1	1:B:121:ARG:HB3	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
1:B:582:GLU:H	1:B:582:GLU:CD	2.16	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:474:LEU:O	1:A:475:HIS:C	2.51	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:O	2:D:326:LEU:HD23	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:LEU:HD12	1:A:537:LEU:H	1.78	0.48
1:A:253:SER:N	1:A:277:ILE:HG12	2.29	0.47
1:B:626:ASN:C	1:B:626:ASN:ND2	2.65	0.47
1:B:546:ALA:HB1	1:B:697:PHE:HB3	1.95	0.47
2:C:258:GLY:C	2:C:259:LYS:HG2	2.33	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: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
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
2:C:96:TYR:H	2:C:207:HIS:HD2	1.64	0.46
1:A:651:ARG:NH2	2:C:356:ASP:OD2	2.48	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
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:397:VAL:C	1:B:399:PRO:HD3	2.35	0.46
1:B:555:PHE:CZ	1:B:594:ALA:HB2	2.50	0.46
2:D:11:VAL:O	2:D:12:SER:HB3	2.15	0.46
1:A:677:ARG:CZ	1:A:750:SER:O	2.64	0.46
2:C:109:MET:CE	2:C:243:LEU:HD21	2.45	0.46
2:C:96:TYR:H	2:C:207:HIS:CD2	2.33	0.46
1:B:165:LEU:HD23	1:B:409:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LEU:O	1:B:475:HIS:C	2.53	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
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: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
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
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: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:CG1	1:A:250:VAL:O	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
1:B:712:LEU:HD23	1:B:712:LEU:C	2.37	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
1:B:319:THR:O	1:B:322:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:543:PRO:O	1:B:547:TYR:HB3	2.16	0.45
1:B:474:LEU:CD1	1:B:550:ILE:HD11	2.46	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:O	2:D:671:LEU:HD13	2.17	0.45
1:A:319:THR:O	1:A:322:PRO:HD3	2.17	0.45
1:A:588:ARG:NH1	1:A:588:ARG:HG2	2.32	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:186:PHE:H	2:C:190:GLY:HA3	1.81	0.45
2:C:52:ILE:HG22	2:C:254:ARG:HG3	1.98	0.45
1:A:202:ILE:HG12	1:A:373:VAL:HG12	1.98	0.44
1:A:537:LEU:N	1:A:537:LEU:HD12	2.32	0.44
1:B:182:TRP:HZ3	1:B:392:VAL:HG12	1.82	0.44
2:C:121:GLY:HA2	2:C:160:PRO:HD2	1.99	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: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:109:MET:HE3	2:C:243:LEU:HD21	1.98	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:408:LEU:HB2	2:C:587:VAL:HB	1.99	0.44
2:C:85:TYR:HE2	2:C:248:SER:HB2	1.83	0.44
1:A:460:SER:OG	1:A:540:ALA:HA	2.17	0.44
1:A:751:GLY:C	1:A:752:ASP:OD1	2.56	0.44
1:B:251:ASN:ND2	1:B:251:ASN:C	2.68	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
2:D:128:TRP:C	2:D:128:TRP:CD1	2.91	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:515:HIS:ND1	1:A:516:PRO:HD2	2.32	0.44
1:A:291:VAL:HA	1:B:524:GLN:O	2.17	0.44
2:C:185:TYR:CD1	2:C:194:CYS:HB2	2.53	0.44
2:C:95:TYR:HE1	2:C:247:PRO:O	2.00	0.44
1:A:165:LEU:O	1:A:169:VAL:HG23	2.18	0.44
1:A:254:ILE:HD12	1:A:373:VAL:HG23	2.00	0.44
1:A:127:LEU:CD2	1:A:442:PHE:CD1	3.01	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: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: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:D:350:HIS:HB2	2:D:629:LEU:HD21	1.99	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:251:ASN:ND2	1:A:251:ASN:C	2.56	0.43
1:A:604:ASP:CG	1:A:605:VAL:H	2.21	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:N	1:B:470:TYR:CD1	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
1:A:604:ASP:CG	1:A:605:VAL:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:603:HIS:CD2	1:A:603:HIS:C	2.93	0.42
1:B:446:ARG:NE	1:B:607:LEU:HD21	2.34	0.42
2:D:599:LYS:HZ2	2:D:600:ILE:HD13	1.82	0.42
2:C:363:VAL:O	2:C:363:VAL:HG12	2.19	0.42
2:C:54:ALA:O	2:C:55:ASN:CG	2.58	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:433:PHE:O	1:B:437:VAL:HG23	2.19	0.42
1:B:186:HIS:CE1	1:B:465:GLU:HB3	2.54	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:O	1:A:496:VAL:HG13	2.19	0.42
1:B:232:LEU:HA	1:B:254:ILE:O	2.20	0.42
2:C:105:SER:H	2:C:232:ARG:HH12	1.67	0.42
2:C:26:MET:O	2:C:30:ILE:HG12	2.19	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
1:A:597:PHE:O	1:A:601:LEU:HD12	2.19	0.42
2:D:380:LYS:O	2:D:383:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:LEU:CD1	1:A:580:ILE:HD12	2.49	0.41
1:A:756:ILE:CG1	1:A:756:ILE:O	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
2:C:19:CYS:O	2:C:22:PHE:HB3	2.20	0.41
2:C:665:CYS:SG	2:C:666:SER:N	2.93	0.41
2:C:45:TYR:CZ	2:C:66:LEU:HD22	2.55	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: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:A:365:MET:C	1:A:366:VAL:HG23	2.40	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:B:474:LEU:C	1:B:474:LEU:HD12	2.40	0.41
1:A:305:THR:HG23	1:A:697:PHE:CZ	2.56	0.41
2:D:145:PRO:HG2	2:D:148:LYS:CB	2.51	0.41
1:A:700:VAL:HB	1:A:709:LEU:CD1	2.51	0.41
1:B:292:ASN:HD21	1:B:294:GLU:C	2.24	0.41
1:B:446:ARG:NH1	1:B:446:ARG:HG3	2.36	0.41
1:B:470:TYR:HB3	1:B:473:SER:HB3	2.02	0.41
1:B:537:LEU:N	1:B:537:LEU:HD12	2.36	0.41
1:A:307:ASP:C	1:A:307:ASP:OD1	2.59	0.40
1:A:565:TYR:CD2	1:A:570:MET:CB	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:263:THR:HG1	1:B:266:GLU:HG3	1.86	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%)	19 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	637/654 (97%)	603 (95%)	32 (5%)	2 (0%)	41 74
2	C	509/693 (73%)	464 (91%)	39 (8%)	6 (1%)	13 48
2	D	467/693 (67%)	434 (93%)	29 (6%)	4 (1%)	17 55
All	All	2249/2694 (84%)	2089 (93%)	143 (6%)	17 (1%)	19 57

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 (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	521/562 (93%)	515 (99%)	6 (1%)	71 87
1	B	483/562 (86%)	477 (99%)	6 (1%)	71 87
2	C	353/585 (60%)	349 (99%)	4 (1%)	73 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	291/585 (50%)	289 (99%)	2 (1%)	84 93
All	All	1648/2294 (72%)	1630 (99%)	18 (1%)	73 88

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
1	A	297	PHE
1	A	357	TRP
1	A	475	HIS
1	A	565	TYR
1	A	753	VAL
1	B	197	GLN
1	B	242	ASP
1	B	251	ASN
1	B	320	GLN
1	B	603	HIS
1	B	626	ASN
2	C	71	TYR
2	C	129	ASN
2	C	241	CYS
2	C	377	CYS
2	D	7	ARG
2	D	383	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	160	GLN
1	A	164	ASN
1	A	251	ASN
1	A	285	GLN
1	A	511	GLN
1	A	512	ASN
1	A	524	GLN
1	A	596	GLN
1	A	603	HIS
1	A	747	ASN
1	A	758	ASN
1	B	148	ASN

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Mol	Chain	Res	Type
1	B	160	GLN
1	B	251	ASN
1	B	285	GLN
1	B	292	ASN
1	B	335	GLN
1	B	483	ASN
1	B	512	ASN
1	B	584	ASN
1	B	596	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	584	ASN
2	C	585	HIS
2	C	604	GLN
2	C	661	ASN
2	D	325	ASN
2	D	383	ASN
2	D	584	ASN
2	D	585	HIS
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	C	905	5	0,3,3	0.00	-	0,3,3	0.00	-
3	NAG	B	903	1	14,14,15	0.42	0	17,19,21	1.17	2 (11%)
3	NAG	A	903	1	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
6	CO3	D	905	5	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	2.27	119.94	116.10
3	A	903	NAG	C8-C7-N2	2.27	119.94	116.10
3	B	903	NAG	C2-N2-C7	-2.06	119.97	122.90
3	A	903	NAG	C2-N2-C7	-2.05	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, 95^{th} 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%)	-0.19	9 (1%) 75 64	45, 81, 127, 200	0
1	B	639/654 (97%)	0.13	27 (4%) 36 24	39, 106, 184, 200	1 (0%)
2	C	515/693 (74%)	0.20	23 (4%) 33 21	71, 127, 182, 200	2 (0%)
2	D	487/693 (70%)	0.44	51 (10%) 6 4	68, 150, 199, 200	1 (0%)
All	All	2279/2694 (84%)	0.12	110 (4%) 30 19	39, 111, 185, 200	4 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	SER	5.2
2	D	288	PRO	5.2
2	D	12	SER	5.2
2	D	613	THR	5.0
2	C	665	CYS	4.9
2	C	33	ASP	4.4
2	D	32	SER	3.9
1	B	210	VAL	3.9
2	D	234	PRO	3.9
2	D	189	SER	3.8
1	A	724	GLY	3.8
2	C	652	GLY	3.8
1	B	751	GLY	3.7
2	C	332	PRO	3.6
2	C	127	GLY	3.4
2	D	240	ASP	3.4
2	D	238	TYR	3.4
2	D	242	HIS	3.3
2	D	86	GLY	3.3
2	C	92	GLN	3.3
2	D	665	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	352	ASP	3.3
1	B	206	ASN	3.3
2	D	643	ASP	3.2
2	D	176	GLY	3.2
1	A	751	GLY	3.2
2	D	241	CYS	3.2
1	B	570	MET	3.2
2	D	142	PRO	3.1
2	D	14	HIS	3.1
2	D	279	SER	3.1
1	B	203	VAL	3.0
1	B	569	THR	3.0
2	D	184	GLN	3.0
1	B	724	GLY	2.9
2	D	90	ASP	2.9
2	D	282	PHE	2.9
1	B	204	ASP	2.9
2	D	108	GLN	2.9
2	D	17	THR	2.9
2	D	278	LYS	2.9
2	D	175	PRO	2.9
1	B	250	VAL	2.9
2	C	271	GLN	2.8
1	B	150	ASN	2.8
2	C	269	GLN	2.8
2	D	43	ALA	2.8
1	A	483	ASN	2.7
1	B	336	THR	2.7
2	D	229	ASP	2.7
2	D	28	SER	2.7
1	B	422	GLY	2.7
2	C	661	ASN	2.7
2	D	390	SER	2.6
2	D	139	LEU	2.6
1	A	194	ASP	2.6
2	D	127	GLY	2.6
2	C	223	TYR	2.6
1	B	235	ALA	2.6
2	C	371	ALA	2.5
2	D	61	THR	2.5
1	B	205	LYS	2.5
2	C	416	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	370	SER	2.5
2	D	140	PRO	2.5
1	A	406	GLY	2.5
2	D	40	VAL	2.5
2	D	181	THR	2.4
2	C	644	ARG	2.4
2	D	239	LYS	2.4
2	C	417	ASN	2.4
2	C	335	PRO	2.4
1	B	249	PRO	2.4
2	C	25	HIS	2.4
2	D	277	ASP	2.3
1	B	419	SER	2.3
2	C	175	PRO	2.3
2	D	332	PRO	2.3
2	D	33	ASP	2.3
2	C	43	ALA	2.3
1	A	722	ASN	2.3
2	C	270	ALA	2.3
2	D	416	ASP	2.3
1	B	251	ASN	2.2
2	D	336	THR	2.2
1	A	196	ALA	2.2
2	D	168	PRO	2.2
2	D	616	SER	2.2
2	D	91	PRO	2.2
2	D	165	THR	2.2
1	B	282	TYR	2.2
2	D	300	HIS	2.2
2	D	20	GLN	2.2
2	C	120	THR	2.2
1	A	669	PHE	2.2
2	C	34	GLY	2.1
2	C	30	ILE	2.1
2	D	41	LYS	2.1
1	B	226	ALA	2.1
1	B	299	GLY	2.1
2	D	182	LEU	2.1
1	B	233	VAL	2.1
1	B	667	ASP	2.1
1	B	247	TYR	2.1
2	D	13	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	35	PRO	2.0
1	B	417	ALA	2.0
2	C	31	PRO	2.0
2	D	97	ALA	2.0
1	B	289	PRO	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 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, 95^{th} 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	A	903	14/15	0.72	0.34	134,134,134,134	0
3	NAG	B	903	14/15	0.80	0.34	154,154,154,154	0
5	FE	D	901	1/1	0.86	0.14	128,128,128,128	0
6	CO3	D	905	4/4	0.93	0.26	163,163,163,163	0
5	FE	C	901	1/1	0.97	0.18	98,98,98,98	0
6	CO3	C	905	4/4	0.98	0.37	78,78,78,78	0
4	CA	B	900	1/1	0.98	0.13	79,79,79,79	0
4	CA	A	900	1/1	0.98	0.23	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.