



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:55 AM UTC

PDB ID : 4C0P / pdb_00004c0p
Title : Unliganded Transportin 3
Authors : Maertens, G.N.; Cook, N.J.; Hare, S.; Cherepanov, P.
Deposited on : 2013-08-06
Resolution : 2.95 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

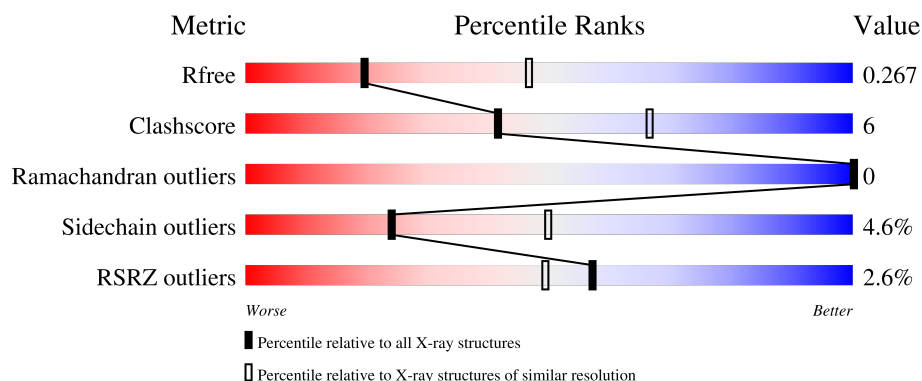
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	923	 2% 76% 19% . .
1	B	923	 3% 77% 18% . .
1	C	923	 3% 77% 18% . .
1	D	923	 2% 77% 18% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28293 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.

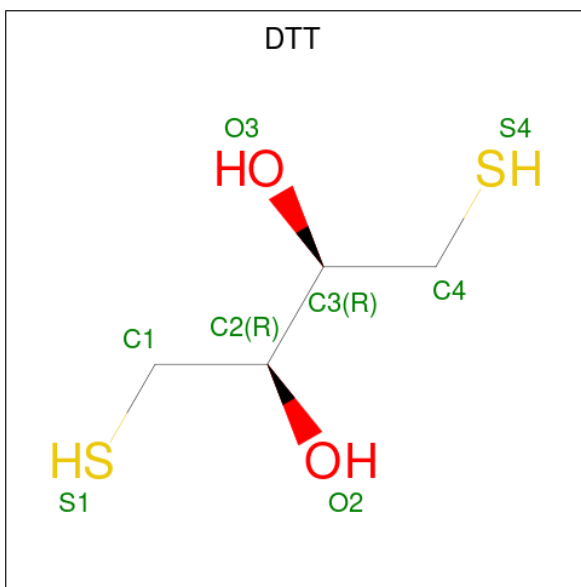
- Molecule 1 is a protein called TRANSPORTIN-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	889	Total	C	N	O	S	0	0	0
			7063	4508	1201	1301	53			
1	B	889	Total	C	N	O	S	0	0	0
			7063	4508	1201	1301	53			
1	C	889	Total	C	N	O	S	0	0	0
			7063	4508	1201	1301	53			
1	D	890	Total	C	N	O	S	0	0	0
			7072	4514	1203	1302	53			

There are 4 discrepancies between the modelled and reference sequences:

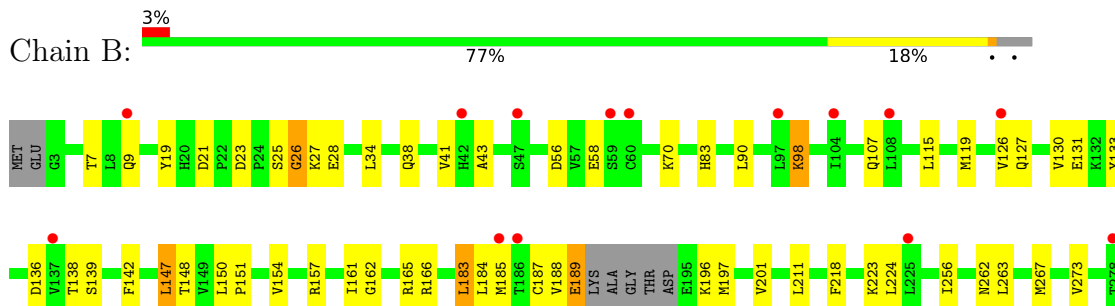
Chain	Residue	Modelled	Actual	Comment	Reference
A	511	ALA	CYS	engineered mutation	UNP Q9Y5L0
B	511	ALA	CYS	engineered mutation	UNP Q9Y5L0
C	511	ALA	CYS	engineered mutation	UNP Q9Y5L0
D	511	ALA	CYS	engineered mutation	UNP Q9Y5L0

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: C₄H₁₀O₂S₂).

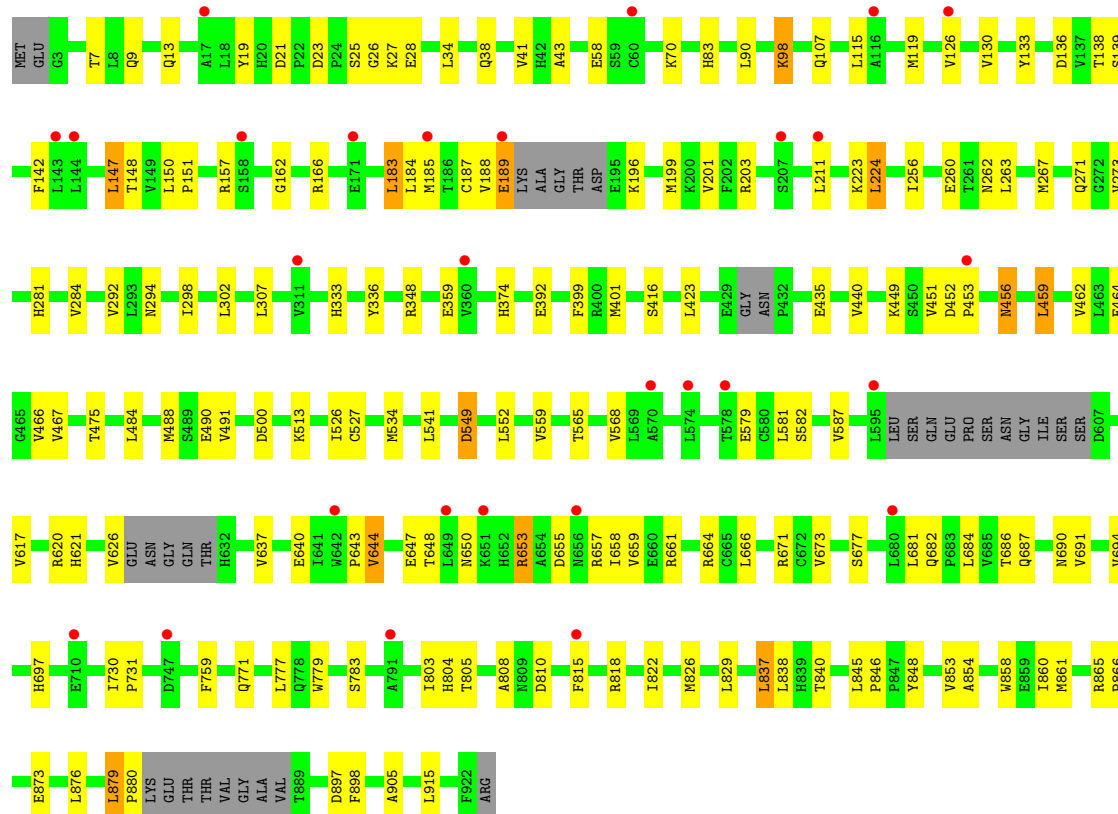
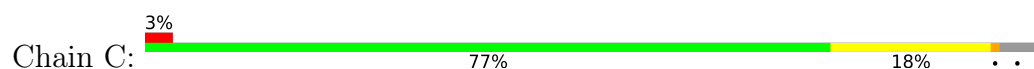


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			8	4	2	2		
2	B	1	Total	C	O	S	0	0
			8	4	2	2		
2	C	1	Total	C	O	S	0	0
			8	4	2	2		
2	D	1	Total	C	O	S	0	0
			8	4	2	2		

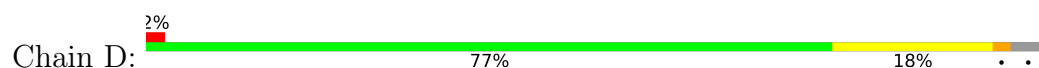
- Molecule 1: TRANSPORTIN-3

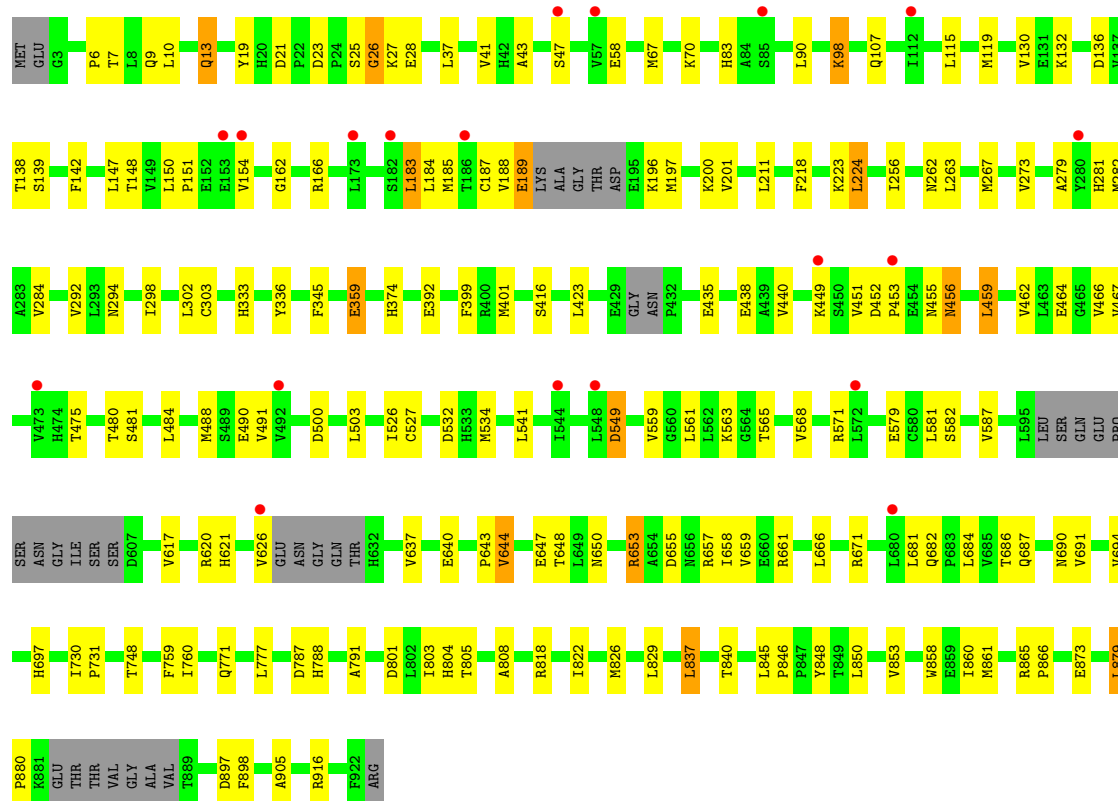


- Molecule 1: TRANSPORTIN-3



- Molecule 1: TRANSPORTIN-3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.20Å 104.02Å 124.89Å 90.64° 97.88° 104.48°	Depositor
Resolution (Å)	38.17 – 2.95 38.17 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.1 (38.17-2.95) 98.5 (38.17-2.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.236 , 0.266 0.238 , 0.267	Depositor DCC
R_{free} test set	4853 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	79.9	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28293	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.28% 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: DTT

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	0.31	0/7203	0.77	4/9779 (0.0%)
1	B	0.32	0/7203	0.76	4/9779 (0.0%)
1	C	0.32	0/7203	0.76	2/9779 (0.0%)
1	D	0.31	0/7212	0.76	4/9790 (0.0%)
All	All	0.31	0/28821	0.76	14/39127 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	ASN	N-CA-C	6.13	117.77	111.14
1	D	452	ASP	CA-C-N	-5.34	114.29	119.90
1	D	452	ASP	C-N-CA	-5.34	114.29	119.90
1	A	452	ASP	CA-C-N	-5.27	114.36	119.90
1	A	452	ASP	C-N-CA	-5.27	114.36	119.90
1	C	452	ASP	CA-C-N	-5.27	114.36	119.90
1	C	452	ASP	C-N-CA	-5.27	114.36	119.90
1	D	26	GLY	N-CA-C	-5.20	106.50	112.73
1	B	26	GLY	N-CA-C	-5.16	106.54	112.73
1	A	26	GLY	N-CA-C	-5.09	106.62	112.73
1	B	452	ASP	CA-C-N	-5.07	114.58	119.90
1	B	452	ASP	C-N-CA	-5.07	114.58	119.90
1	D	218	PHE	CB-CA-C	-5.06	102.39	110.79
1	B	218	PHE	CB-CA-C	-5.00	102.48	110.79

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	7063	0	7102	93	0
1	B	7063	0	7102	91	0
1	C	7063	0	7102	87	0
1	D	7072	0	7115	96	0
2	A	8	0	10	3	0
2	B	8	0	10	1	0
2	C	8	0	10	1	0
2	D	8	0	10	0	0
All	All	28293	0	28461	365	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 6.

All (365) 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:826:MET:HE1	1:B:860:ILE:HG23	1.58	0.85
1:D:21:ASP:O	1:D:27:LYS:NZ	2.09	0.85
1:D:826:MET:HE1	1:D:860:ILE:HG23	1.59	0.84
1:B:21:ASP:O	1:B:27:LYS:NZ	2.10	0.83
1:A:21:ASP:O	1:A:27:LYS:NZ	2.10	0.83
1:C:21:ASP:O	1:C:27:LYS:NZ	2.12	0.81
1:B:151:PRO:HB3	1:B:211:LEU:HD23	1.64	0.80
1:A:826:MET:HE1	1:A:860:ILE:HG23	1.69	0.74
1:D:184:LEU:HG	1:D:201:VAL:HG13	1.71	0.73
1:A:184:LEU:HG	1:A:201:VAL:HG13	1.71	0.72
1:D:541:LEU:HB3	1:D:565:THR:HG22	1.71	0.72
1:C:151:PRO:HB3	1:C:211:LEU:HD23	1.72	0.72
1:C:541:LEU:HB3	1:C:565:THR:HG22	1.71	0.72
1:C:826:MET:HE1	1:C:860:ILE:HG23	1.69	0.72
1:D:151:PRO:HB3	1:D:211:LEU:HD23	1.72	0.71
1:B:541:LEU:HB3	1:B:565:THR:HG22	1.73	0.71
1:A:541:LEU:HB3	1:A:565:THR:HG22	1.72	0.69
1:B:526:ILE:HG22	1:B:534:MET:HE1	1.74	0.69
1:B:184:LEU:HG	1:B:201:VAL:HG13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:LEU:HB2	1:D:491:VAL:HG21	1.76	0.68
1:A:151:PRO:HB3	1:A:211:LEU:HD23	1.76	0.67
1:A:281:HIS:HA	1:A:284:VAL:HG12	1.78	0.66
1:C:526:ILE:HG22	1:C:534:MET:HE1	1.77	0.66
1:B:273:VAL:HG11	1:B:302:LEU:HD13	1.78	0.66
1:B:459:LEU:HB2	1:B:491:VAL:HG21	1.78	0.66
1:C:184:LEU:HG	1:C:201:VAL:HG13	1.77	0.65
1:A:459:LEU:HB2	1:A:491:VAL:HG21	1.77	0.65
1:D:865:ARG:NH2	1:D:905:ALA:O	2.29	0.65
1:A:526:ILE:HG22	1:A:534:MET:HE1	1.77	0.65
1:B:549:ASP:OD1	1:B:549:ASP:N	2.29	0.64
1:D:526:ILE:HG22	1:D:534:MET:HE1	1.79	0.64
1:D:281:HIS:HA	1:D:284:VAL:HG12	1.80	0.63
1:B:23:ASP:OD1	1:B:26:GLY:N	2.25	0.63
1:C:273:VAL:HG11	1:C:302:LEU:HD13	1.82	0.62
1:A:664:ARG:HH11	2:A:1923:DTT:H42	1.64	0.62
1:A:865:ARG:NH2	1:A:905:ALA:O	2.33	0.62
1:C:281:HIS:HA	1:C:284:VAL:HG12	1.81	0.62
1:B:256:ILE:HG23	1:B:262:ASN:HD22	1.65	0.61
1:C:549:ASP:OD1	1:C:549:ASP:N	2.33	0.61
1:D:549:ASP:OD1	1:D:549:ASP:N	2.32	0.61
1:C:256:ILE:HG23	1:C:262:ASN:HD22	1.64	0.61
1:D:23:ASP:OD1	1:D:26:GLY:N	2.27	0.61
1:A:23:ASP:OD1	1:A:26:GLY:N	2.27	0.61
1:B:281:HIS:HA	1:B:284:VAL:HG12	1.82	0.61
1:B:686:THR:O	1:B:690:ASN:ND2	2.34	0.61
1:A:400:ARG:NH2	1:A:438:GLU:OE2	2.33	0.60
1:C:865:ARG:NH2	1:C:905:ALA:O	2.34	0.60
1:D:273:VAL:HG11	1:D:302:LEU:HD13	1.82	0.60
1:C:459:LEU:HB2	1:C:491:VAL:HG21	1.82	0.60
1:C:43:ALA:HB3	1:C:70:LYS:HD2	1.83	0.60
1:B:263:LEU:HD22	1:B:267:MET:HE3	1.84	0.60
1:B:581:LEU:HG	1:B:637:VAL:HG11	1.84	0.60
1:C:837:LEU:HG	1:C:853:VAL:HG13	1.83	0.60
1:A:805:THR:HB	1:A:822:ILE:HD11	1.84	0.60
1:B:865:ARG:NH2	1:B:905:ALA:O	2.35	0.60
1:A:273:VAL:HG11	1:A:302:LEU:HD13	1.84	0.59
1:A:453:PRO:HB2	1:A:456:ASN:HD21	1.67	0.59
1:A:549:ASP:OD1	1:A:549:ASP:N	2.35	0.59
1:C:453:PRO:HB2	1:C:456:ASN:HD21	1.67	0.59
1:D:43:ALA:HB3	1:D:70:LYS:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ALA:HB3	1:B:70:LYS:HD2	1.85	0.58
1:D:453:PRO:HB2	1:D:456:ASN:HD21	1.68	0.58
1:D:686:THR:O	1:D:690:ASN:ND2	2.37	0.58
1:C:23:ASP:OD1	1:C:26:GLY:N	2.26	0.57
1:A:256:ILE:HG23	1:A:262:ASN:HD22	1.70	0.57
1:C:189:GLU:OE2	1:C:223:LYS:NZ	2.38	0.57
1:D:532:ASP:OD1	1:D:571:ARG:NH1	2.38	0.57
1:C:19:TYR:HD2	1:C:58:GLU:HG2	1.70	0.56
1:D:19:TYR:HD2	1:D:58:GLU:HG2	1.69	0.56
1:D:858:TRP:HA	1:D:861:MET:HE3	1.88	0.56
1:B:453:PRO:HB2	1:B:456:ASN:HD21	1.69	0.56
1:D:256:ILE:HG23	1:D:262:ASN:HD22	1.69	0.56
1:A:687:GLN:O	1:A:691:VAL:HG12	2.06	0.56
1:D:534:MET:HG2	1:D:568:VAL:HG11	1.87	0.56
1:A:130:VAL:HG23	1:A:183:LEU:HD13	1.88	0.55
1:A:686:THR:O	1:A:690:ASN:ND2	2.39	0.55
1:B:687:GLN:O	1:B:691:VAL:HG12	2.06	0.55
1:B:19:TYR:HD2	1:B:58:GLU:HG2	1.72	0.55
1:D:189:GLU:OE2	1:D:223:LYS:NZ	2.38	0.55
1:A:19:TYR:HD2	1:A:58:GLU:HG2	1.72	0.55
1:C:644:VAL:O	1:C:648:THR:OG1	2.22	0.55
1:C:686:THR:O	1:C:690:ASN:ND2	2.39	0.55
1:D:659:VAL:HG11	1:D:697:HIS:CD2	2.42	0.54
1:C:687:GLN:O	1:C:691:VAL:HG12	2.08	0.54
1:B:423:LEU:HB3	1:B:440:VAL:HG13	1.89	0.54
1:A:532:ASP:OD1	1:A:571:ARG:NH1	2.40	0.54
1:C:534:MET:HG2	1:C:568:VAL:HG11	1.89	0.54
1:B:136:ASP:O	1:B:138:THR:N	2.39	0.54
1:A:90:LEU:HD12	1:A:115:LEU:HD22	1.89	0.54
1:B:659:VAL:HG11	1:B:697:HIS:CD2	2.43	0.54
1:C:659:VAL:HG11	1:C:697:HIS:CD2	2.43	0.54
1:B:83:HIS:HB3	1:B:119:MET:HE2	1.90	0.53
1:C:90:LEU:HD12	1:C:115:LEU:HD22	1.89	0.53
1:C:664:ARG:HH11	2:C:1923:DTT:H41	1.72	0.53
1:A:659:VAL:HG11	1:A:697:HIS:CD2	2.44	0.53
1:C:136:ASP:O	1:C:138:THR:N	2.39	0.53
1:C:858:TRP:HA	1:C:861:MET:HE3	1.91	0.53
1:C:83:HIS:HB3	1:C:119:MET:HE2	1.91	0.52
1:B:189:GLU:OE2	1:B:223:LYS:NZ	2.40	0.52
1:B:534:MET:HG2	1:B:568:VAL:HG11	1.90	0.52
1:A:43:ALA:HB3	1:A:70:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:VAL:O	1:B:648:THR:OG1	2.24	0.52
1:A:83:HIS:HB3	1:A:119:MET:HE2	1.92	0.52
1:D:130:VAL:HG23	1:D:183:LEU:HD13	1.92	0.52
1:D:620:ARG:HD3	1:D:621:HIS:CE1	2.45	0.51
1:B:897:ASP:OD1	1:B:898:PHE:N	2.44	0.51
1:D:897:ASP:OD1	1:D:898:PHE:N	2.44	0.51
1:A:897:ASP:OD1	1:A:898:PHE:N	2.44	0.51
1:D:162:GLY:O	1:D:166:ARG:NH1	2.43	0.51
1:D:687:GLN:O	1:D:691:VAL:HG12	2.10	0.51
1:C:126:VAL:HG13	1:C:147:LEU:HD11	1.93	0.51
1:C:897:ASP:OD1	1:C:898:PHE:N	2.43	0.51
1:A:423:LEU:HB3	1:A:440:VAL:HG13	1.93	0.51
1:A:650:ASN:O	1:A:653:ARG:HD2	2.11	0.51
1:A:664:ARG:NH1	2:A:1923:DTT:H42	2.26	0.51
1:C:7:THR:HG22	1:C:9:GLN:H	1.74	0.51
1:A:136:ASP:O	1:A:138:THR:N	2.40	0.51
1:C:488:MET:HE2	1:C:491:VAL:HG11	1.93	0.51
1:B:532:ASP:OD1	1:B:571:ARG:NH1	2.44	0.50
1:C:666:LEU:HD22	1:C:684:LEU:HD13	1.93	0.50
1:D:90:LEU:HD12	1:D:115:LEU:HD22	1.93	0.50
1:B:98:LYS:HG3	1:B:142:PHE:HD2	1.77	0.50
1:B:162:GLY:O	1:B:166:ARG:NH1	2.44	0.50
1:B:803:ILE:HD11	1:B:833:LEU:HD21	1.93	0.50
1:C:392:GLU:HG2	1:C:401:MET:HE3	1.93	0.50
1:B:130:VAL:HG23	1:B:183:LEU:HD13	1.93	0.50
1:C:579:GLU:O	1:C:582:SER:OG	2.26	0.50
1:A:392:GLU:HG2	1:A:401:MET:HE3	1.92	0.50
1:C:650:ASN:O	1:C:653:ARG:HD2	2.11	0.50
1:B:653:ARG:HB2	1:B:691:VAL:HG23	1.94	0.49
1:C:620:ARG:HD3	1:C:621:HIS:CE1	2.46	0.49
1:B:620:ARG:HD3	1:B:621:HIS:CE1	2.47	0.49
1:C:527:CYS:HA	1:C:534:MET:HE3	1.93	0.49
1:D:488:MET:HE2	1:D:491:VAL:HG11	1.93	0.49
1:D:771:GLN:OE1	1:D:771:GLN:N	2.45	0.49
1:B:559:VAL:HG13	1:B:617:VAL:HG21	1.95	0.49
1:C:294:ASN:O	1:C:298:ILE:HG13	2.13	0.49
1:C:653:ARG:HB2	1:C:691:VAL:HG23	1.94	0.49
1:C:777:LEU:HD23	1:C:829:LEU:HD12	1.94	0.49
1:A:760:ILE:HG21	1:A:801:ASP:HB3	1.95	0.49
1:B:858:TRP:HA	1:B:861:MET:HE3	1.94	0.49
1:A:559:VAL:HG13	1:A:617:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:LEU:HD22	1:B:684:LEU:HD13	1.93	0.49
1:A:292:VAL:HG21	1:A:333:HIS:CD2	2.48	0.49
1:D:83:HIS:HB3	1:D:119:MET:HE2	1.93	0.49
1:D:666:LEU:HD22	1:D:684:LEU:HD13	1.94	0.49
1:A:98:LYS:HG3	1:A:142:PHE:HD2	1.78	0.48
1:B:805:THR:HB	1:B:822:ILE:HD11	1.94	0.48
1:A:579:GLU:O	1:A:582:SER:OG	2.30	0.48
1:C:581:LEU:HG	1:C:637:VAL:HG11	1.94	0.48
1:A:7:THR:HG22	1:A:9:GLN:H	1.78	0.48
1:D:292:VAL:HG21	1:D:333:HIS:CD2	2.49	0.48
1:D:804:HIS:NE2	1:D:808:ALA:HB2	2.28	0.48
1:A:846:PRO:HB2	1:A:848:TYR:CD1	2.48	0.48
1:D:650:ASN:O	1:D:653:ARG:HD2	2.14	0.48
1:C:98:LYS:HG3	1:C:142:PHE:HD2	1.79	0.48
1:D:136:ASP:O	1:D:138:THR:N	2.40	0.48
1:B:771:GLN:OE1	1:B:771:GLN:N	2.45	0.48
1:B:837:LEU:HG	1:B:853:VAL:HG13	1.95	0.48
1:D:644:VAL:O	1:D:648:THR:OG1	2.29	0.48
1:B:804:HIS:NE2	1:B:808:ALA:HB2	2.29	0.48
1:A:534:MET:HG2	1:A:568:VAL:HG11	1.96	0.47
1:B:148:THR:O	1:B:151:PRO:HD2	2.14	0.47
1:B:307:LEU:HD13	1:B:348:ARG:NH1	2.30	0.47
1:A:150:LEU:HB3	1:A:151:PRO:HD3	1.96	0.47
1:A:804:HIS:NE2	1:A:808:ALA:HB2	2.29	0.47
1:B:527:CYS:HA	1:B:534:MET:HE3	1.97	0.47
1:D:150:LEU:HB3	1:D:151:PRO:HD3	1.96	0.47
1:D:416:SER:HB2	1:D:451:VAL:HG22	1.95	0.47
1:D:423:LEU:HB3	1:D:440:VAL:HG13	1.95	0.47
1:D:657:ARG:O	1:D:661:ARG:HG2	2.14	0.47
1:B:392:GLU:HG2	1:B:401:MET:HE3	1.97	0.47
1:C:846:PRO:HB2	1:C:848:TYR:CD1	2.50	0.47
1:D:197:MET:O	1:D:197:MET:HG3	2.15	0.47
1:D:392:GLU:HG2	1:D:401:MET:HE3	1.96	0.47
1:D:438:GLU:OE2	1:D:480:THR:HG21	2.15	0.47
1:B:805:THR:O	1:B:818:ARG:NH1	2.45	0.47
1:A:527:CYS:HA	1:A:534:MET:HE3	1.96	0.47
1:A:771:GLN:OE1	1:A:771:GLN:N	2.44	0.47
1:B:579:GLU:O	1:B:582:SER:OG	2.30	0.47
1:B:846:PRO:HB2	1:B:848:TYR:CD1	2.50	0.47
1:B:367:ALA:HA	1:B:370:GLN:HE21	1.79	0.47
1:C:513:LYS:HD2	1:C:552:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:VAL:HG23	1:C:183:LEU:HD13	1.97	0.46
1:B:803:ILE:HD13	1:B:860:ILE:HG12	1.97	0.46
1:C:148:THR:O	1:C:151:PRO:HD2	2.15	0.46
1:C:771:GLN:OE1	1:C:771:GLN:N	2.44	0.46
1:B:197:MET:HG3	1:B:197:MET:O	2.15	0.46
1:D:803:ILE:HD13	1:D:860:ILE:HG12	1.96	0.46
1:D:805:THR:HB	1:D:822:ILE:HD11	1.97	0.46
1:A:803:ILE:HD11	1:A:833:LEU:HD21	1.97	0.46
1:A:899:HIS:CE1	1:A:903:THR:HG21	2.51	0.46
1:B:7:THR:HG22	1:B:9:GLN:H	1.79	0.46
1:C:423:LEU:HB3	1:C:440:VAL:HG13	1.97	0.46
1:C:730:ILE:HB	1:C:731:PRO:HD3	1.98	0.46
1:C:805:THR:HG22	1:C:818:ARG:HD2	1.98	0.46
1:D:148:THR:O	1:D:151:PRO:HD2	2.15	0.46
1:D:805:THR:HG22	1:D:818:ARG:HD2	1.97	0.46
1:A:279:ALA:HA	1:A:282:MET:HE3	1.97	0.46
1:B:126:VAL:HG13	1:B:147:LEU:HD11	1.97	0.46
1:C:673:VAL:HB	1:C:677:SER:HB3	1.98	0.46
1:B:150:LEU:HB3	1:B:151:PRO:HD3	1.97	0.46
1:A:811:HIS:HB3	1:D:671:ARG:NH2	2.31	0.46
1:D:846:PRO:HB2	1:D:848:TYR:CD1	2.50	0.46
1:C:803:ILE:HD13	1:C:860:ILE:HG12	1.97	0.46
1:A:126:VAL:HG13	1:A:147:LEU:HD11	1.98	0.46
1:B:289:LEU:HA	1:B:292:VAL:HG12	1.98	0.46
1:A:777:LEU:HD23	1:A:829:LEU:HD12	1.98	0.45
1:C:810:ASP:HA	1:C:815:PHE:CG	2.51	0.45
1:D:640:GLU:O	1:D:643:PRO:HD2	2.16	0.45
1:A:185:MET:O	1:A:188:VAL:HG22	2.17	0.45
1:B:466:VAL:HG13	1:B:481:SER:HB2	1.97	0.45
1:C:488:MET:O	1:C:491:VAL:HG12	2.16	0.45
1:D:10:LEU:HA	1:D:13:GLN:HB2	1.97	0.45
1:D:185:MET:O	1:D:188:VAL:HG22	2.16	0.45
1:D:837:LEU:HD12	1:D:837:LEU:HA	1.84	0.45
1:A:162:GLY:O	1:A:166:ARG:NH1	2.49	0.45
1:B:151:PRO:O	1:B:154:VAL:HG12	2.17	0.45
1:B:464:GLU:HA	1:B:467:VAL:HG22	1.99	0.45
1:C:464:GLU:HA	1:C:467:VAL:HG22	1.97	0.45
1:C:559:VAL:HG13	1:C:617:VAL:HG21	1.99	0.45
1:D:559:VAL:HG13	1:D:617:VAL:HG21	1.99	0.45
1:D:730:ILE:HB	1:D:731:PRO:HD3	1.99	0.45
1:C:150:LEU:HB3	1:C:151:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:TYR:HB2	1:C:399:PHE:CZ	2.51	0.45
1:D:464:GLU:HA	1:D:467:VAL:HG22	1.99	0.45
1:D:840:THR:HG23	1:D:845:LEU:HG	1.99	0.45
1:A:803:ILE:HD13	1:A:860:ILE:HG12	1.99	0.45
1:A:464:GLU:HA	1:A:467:VAL:HG22	1.99	0.45
1:B:484:LEU:O	1:B:488:MET:HG3	2.17	0.45
1:D:47:SER:HB3	1:D:67:MET:HG2	1.99	0.45
1:A:644:VAL:O	1:A:648:THR:OG1	2.28	0.44
1:A:703:LEU:HB2	2:A:1923:DTT:S1	2.57	0.44
1:C:805:THR:O	1:C:818:ARG:NH1	2.48	0.44
1:B:90:LEU:HD12	1:B:115:LEU:HD22	1.99	0.44
1:B:462:VAL:O	1:B:466:VAL:HG23	2.17	0.44
1:A:336:TYR:HB2	1:A:399:PHE:CZ	2.52	0.44
1:A:148:THR:O	1:A:151:PRO:HD2	2.17	0.44
1:C:34:LEU:O	1:C:38:GLN:HG3	2.18	0.44
1:D:527:CYS:HA	1:D:534:MET:HE3	1.99	0.44
1:A:303:CYS:HB3	1:A:345:PHE:CE1	2.53	0.44
1:B:655:ASP:OD1	1:B:658:ILE:HG12	2.18	0.44
1:D:294:ASN:O	1:D:298:ILE:HG13	2.18	0.44
1:A:488:MET:O	1:A:491:VAL:HG12	2.17	0.44
1:A:620:ARG:HD3	1:A:621:HIS:CE1	2.53	0.44
1:A:726:GLN:HG2	1:A:772:VAL:HB	2.00	0.44
1:D:760:ILE:HG21	1:D:801:ASP:HB3	2.00	0.44
1:C:185:MET:O	1:C:188:VAL:HG22	2.18	0.44
1:C:804:HIS:NE2	1:C:808:ALA:HB2	2.33	0.44
1:D:655:ASP:OD1	1:D:658:ILE:HG12	2.18	0.44
1:C:838:LEU:HD21	1:C:876:LEU:HD23	2.00	0.43
1:C:879:LEU:HA	1:C:880:PRO:HD3	1.87	0.43
1:B:787:ASP:HA	1:B:845:LEU:HD22	2.00	0.43
1:C:224:LEU:HD12	1:C:224:LEU:HA	1.78	0.43
1:A:484:LEU:O	1:A:488:MET:HG3	2.18	0.43
1:B:488:MET:O	1:B:491:VAL:HG12	2.18	0.43
1:B:640:GLU:O	1:B:643:PRO:HD2	2.18	0.43
1:A:459:LEU:H	1:A:459:LEU:HG	1.62	0.43
1:A:657:ARG:O	1:A:661:ARG:HG2	2.18	0.43
1:B:811:HIS:HB3	1:C:671:ARG:NH2	2.33	0.43
1:D:777:LEU:HD23	1:D:829:LEU:HD12	1.99	0.43
1:D:837:LEU:HG	1:D:853:VAL:HG13	2.00	0.43
1:B:837:LEU:HD12	1:B:837:LEU:HA	1.89	0.43
1:A:837:LEU:HD12	1:A:837:LEU:HA	1.87	0.43
1:C:655:ASP:OD1	1:C:658:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:THR:HG22	1:D:9:GLN:H	1.83	0.43
1:A:858:TRP:HA	1:A:861:MET:HE3	2.00	0.43
1:D:879:LEU:HA	1:D:880:PRO:HD3	1.87	0.43
1:A:10:LEU:HA	1:A:13:GLN:HB2	2.00	0.43
1:C:854:ALA:HB2	1:C:915:LEU:HD12	2.00	0.43
1:D:98:LYS:HG3	1:D:142:PHE:HD2	1.84	0.43
1:D:336:TYR:HB2	1:D:399:PHE:CZ	2.54	0.43
1:A:655:ASP:OD1	1:A:658:ILE:HG12	2.18	0.43
1:B:730:ILE:HB	1:B:731:PRO:HD3	2.00	0.43
1:B:850:LEU:HD13	1:B:916:ARG:HA	2.00	0.43
1:A:151:PRO:O	1:A:154:VAL:HG12	2.19	0.43
1:A:466:VAL:HG13	1:A:481:SER:HB2	2.01	0.43
1:C:779:TRP:O	1:C:783:SER:OG	2.36	0.43
1:A:56:ASP:HB3	1:A:58:GLU:OE1	2.19	0.42
1:B:810:ASP:HA	1:B:815:PHE:CG	2.54	0.42
1:C:263:LEU:HD22	1:C:267:MET:HE3	2.01	0.42
1:C:162:GLY:O	1:C:166:ARG:NH1	2.52	0.42
1:D:563:LYS:HE3	1:D:621:HIS:NE2	2.34	0.42
1:A:462:VAL:O	1:A:466:VAL:HG23	2.20	0.42
1:B:56:ASP:HB3	1:B:58:GLU:OE1	2.19	0.42
1:B:459:LEU:H	1:B:459:LEU:HG	1.67	0.42
1:C:133:TYR:O	1:C:139:SER:OG	2.37	0.42
1:C:416:SER:HB2	1:C:451:VAL:HG22	2.01	0.42
1:A:854:ALA:HB2	1:A:915:LEU:HD12	2.00	0.42
1:B:185:MET:O	1:B:188:VAL:HG22	2.20	0.42
1:C:462:VAL:O	1:C:466:VAL:HG23	2.20	0.42
1:A:561:LEU:O	1:A:565:THR:HG23	2.20	0.42
1:A:730:ILE:HB	1:A:731:PRO:HD3	2.01	0.42
1:B:760:ILE:HG21	1:B:801:ASP:HB3	2.02	0.42
1:D:263:LEU:HD22	1:D:267:MET:HE3	2.00	0.42
1:C:307:LEU:HD13	1:C:348:ARG:NH1	2.35	0.42
1:D:488:MET:O	1:D:491:VAL:HG12	2.19	0.42
1:A:810:ASP:HA	1:A:815:PHE:CG	2.55	0.42
1:C:657:ARG:O	1:C:661:ARG:HG2	2.20	0.42
1:D:303:CYS:HB3	1:D:345:PHE:CE1	2.55	0.42
1:A:481:SER:O	1:A:485:VAL:HG23	2.20	0.41
1:B:637:VAL:O	1:B:641:ILE:HG13	2.20	0.41
1:B:840:THR:HG23	1:B:845:LEU:HG	2.02	0.41
1:D:787:ASP:HA	1:D:845:LEU:HD22	2.01	0.41
1:D:200:LYS:HA	1:D:200:LYS:HD3	1.82	0.41
1:D:279:ALA:HA	1:D:282:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:653:ARG:HB2	1:D:691:VAL:HG23	2.02	0.41
1:A:637:VAL:O	1:A:641:ILE:HG13	2.20	0.41
1:B:416:SER:HB2	1:B:451:VAL:HG22	2.01	0.41
1:B:653:ARG:NH2	1:B:694:VAL:HG11	2.35	0.41
1:A:256:ILE:HD11	1:A:269:LEU:HD12	2.02	0.41
1:A:294:ASN:O	1:A:298:ILE:HG13	2.20	0.41
1:A:709:ASP:HB2	1:A:758:ARG:HG3	2.01	0.41
1:B:133:TYR:O	1:B:139:SER:OG	2.38	0.41
1:C:260:GLU:HA	1:C:263:LEU:HG	2.02	0.41
1:D:804:HIS:CD2	1:D:808:ALA:HB2	2.56	0.41
1:D:865:ARG:N	1:D:866:PRO:HD2	2.36	0.41
1:D:151:PRO:O	1:D:154:VAL:HG12	2.21	0.41
1:D:359:GLU:CD	1:D:359:GLU:H	2.29	0.41
1:D:563:LYS:HE3	1:D:621:HIS:CD2	2.56	0.41
1:A:98:LYS:HZ1	1:A:105:VAL:HG11	1.86	0.41
1:C:846:PRO:HB2	1:C:848:TYR:HD1	1.85	0.41
1:C:292:VAL:HG21	1:C:333:HIS:CD2	2.56	0.41
1:C:810:ASP:HA	1:C:815:PHE:CD1	2.56	0.41
1:D:455:ASN:OD1	1:D:455:ASN:N	2.54	0.41
1:C:199:MET:O	1:C:203:ARG:HG3	2.21	0.41
1:C:822:ILE:HG23	1:C:826:MET:HG3	2.02	0.41
1:D:655:ASP:CG	1:D:658:ILE:HG12	2.46	0.41
1:A:569:LEU:HD22	1:A:584:LEU:HD13	2.03	0.41
1:A:728:LEU:O	1:A:732:THR:OG1	2.22	0.41
1:B:899:HIS:CE1	1:B:903:THR:HG21	2.55	0.41
1:D:130:VAL:C	1:D:132:LYS:H	2.29	0.41
1:D:224:LEU:HD12	1:D:224:LEU:HA	1.83	0.41
1:D:503:LEU:HD11	1:D:534:MET:SD	2.61	0.41
1:D:579:GLU:O	1:D:582:SER:OG	2.36	0.41
1:D:788:HIS:HB3	1:D:791:ALA:HB3	2.02	0.41
1:A:788:HIS:HB3	1:A:791:ALA:HB3	2.01	0.41
1:B:667:ARG:HG2	2:B:1923:DTT:H41	2.03	0.41
1:B:838:LEU:HD21	1:B:876:LEU:HD23	2.02	0.41
1:A:197:MET:O	1:A:197:MET:HG3	2.19	0.40
1:D:850:LEU:HD13	1:D:916:ARG:HA	2.02	0.40
1:B:303:CYS:HB3	1:B:345:PHE:CZ	2.57	0.40
1:C:840:THR:HG23	1:C:845:LEU:HG	2.04	0.40
1:A:119:MET:SD	1:A:122:TRP:HB2	2.62	0.40
1:A:294:ASN:OD1	1:A:297:ARG:NH1	2.54	0.40
1:A:787:ASP:HA	1:A:845:LEU:HD22	2.04	0.40
1:B:161:ILE:HG13	1:B:165:ARG:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:MET:HE2	1:B:534:MET:HB2	1.91	0.40
1:B:561:LEU:HD12	1:B:561:LEU:HA	1.82	0.40
1:D:466:VAL:HG13	1:D:481:SER:HB2	2.02	0.40
1:D:561:LEU:O	1:D:565:THR:HG23	2.20	0.40
1:A:640:GLU:O	1:A:643:PRO:HD2	2.22	0.40
1:A:760:ILE:HD13	1:A:760:ILE:HA	1.89	0.40
1:B:34:LEU:O	1:B:38:GLN:HG3	2.21	0.40
1:C:640:GLU:O	1:C:643:PRO:HD2	2.22	0.40
1:D:6:PRO:HG2	1:D:37:LEU:HD13	2.02	0.40
1:D:462:VAL:O	1:D:466:VAL:HG23	2.21	0.40
1:A:438:GLU:OE2	1:A:480:THR:HG21	2.22	0.40
1:B:127:GLN:O	1:B:131:GLU:HG2	2.21	0.40
1:B:303:CYS:HB3	1:B:345:PHE:CE1	2.56	0.40
1:B:865:ARG:N	1:B:866:PRO:HD2	2.36	0.40
1:C:804:HIS:CD2	1:C:808:ALA:HB2	2.57	0.40
1:C:865:ARG:N	1:C:866:PRO:HD2	2.37	0.40
1:D:136:ASP:HB3	1:D:139:SER:OG	2.21	0.40
1:D:581:LEU:HG	1:D:637:VAL:HG11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	877/923 (95%)	847 (97%)	30 (3%)	0	100	100
1	B	877/923 (95%)	847 (97%)	30 (3%)	0	100	100
1	C	877/923 (95%)	848 (97%)	29 (3%)	0	100	100
1	D	878/923 (95%)	847 (96%)	31 (4%)	0	100	100
All	All	3509/3692 (95%)	3389 (97%)	120 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	793/820 (97%)	757 (96%)	36 (4%)	24	50
1	B	793/820 (97%)	756 (95%)	37 (5%)	23	49
1	C	793/820 (97%)	756 (95%)	37 (5%)	23	49
1	D	794/820 (97%)	758 (96%)	36 (4%)	24	50
All	All	3173/3280 (97%)	3027 (95%)	146 (5%)	24	50

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	28	GLU
1	A	41	VAL
1	A	98	LYS
1	A	107	GLN
1	A	147	LEU
1	A	157	ARG
1	A	183	LEU
1	A	187	CYS
1	A	189	GLU
1	A	196	LYS
1	A	224	LEU
1	A	359	GLU
1	A	374	HIS
1	A	435	GLU
1	A	449	LYS
1	A	456	ASN
1	A	459	LEU
1	A	475	THR
1	A	484	LEU
1	A	490	GLU
1	A	500	ASP
1	A	549	ASP
1	A	587	VAL

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Mol	Chain	Res	Type
1	A	626	VAL
1	A	644	VAL
1	A	647	GLU
1	A	653	ARG
1	A	681	LEU
1	A	682	GLN
1	A	694	VAL
1	A	748	THR
1	A	759	PHE
1	A	837	LEU
1	A	873	GLU
1	A	879	LEU
1	B	25	SER
1	B	28	GLU
1	B	41	VAL
1	B	98	LYS
1	B	107	GLN
1	B	147	LEU
1	B	157	ARG
1	B	183	LEU
1	B	187	CYS
1	B	189	GLU
1	B	196	LYS
1	B	224	LEU
1	B	359	GLU
1	B	374	HIS
1	B	435	GLU
1	B	449	LYS
1	B	456	ASN
1	B	459	LEU
1	B	475	THR
1	B	484	LEU
1	B	490	GLU
1	B	500	ASP
1	B	549	ASP
1	B	587	VAL
1	B	626	VAL
1	B	644	VAL
1	B	647	GLU
1	B	650	ASN
1	B	653	ARG
1	B	681	LEU

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Mol	Chain	Res	Type
1	B	682	GLN
1	B	694	VAL
1	B	748	THR
1	B	759	PHE
1	B	837	LEU
1	B	873	GLU
1	B	879	LEU
1	C	13	GLN
1	C	25	SER
1	C	28	GLU
1	C	41	VAL
1	C	98	LYS
1	C	107	GLN
1	C	147	LEU
1	C	157	ARG
1	C	183	LEU
1	C	187	CYS
1	C	189	GLU
1	C	196	LYS
1	C	224	LEU
1	C	271	GLN
1	C	359	GLU
1	C	374	HIS
1	C	435	GLU
1	C	449	LYS
1	C	456	ASN
1	C	459	LEU
1	C	475	THR
1	C	484	LEU
1	C	490	GLU
1	C	500	ASP
1	C	549	ASP
1	C	587	VAL
1	C	626	VAL
1	C	644	VAL
1	C	647	GLU
1	C	653	ARG
1	C	681	LEU
1	C	682	GLN
1	C	694	VAL
1	C	759	PHE
1	C	837	LEU

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Mol	Chain	Res	Type
1	C	873	GLU
1	C	879	LEU
1	D	13	GLN
1	D	25	SER
1	D	28	GLU
1	D	41	VAL
1	D	98	LYS
1	D	107	GLN
1	D	147	LEU
1	D	183	LEU
1	D	187	CYS
1	D	189	GLU
1	D	196	LYS
1	D	224	LEU
1	D	359	GLU
1	D	374	HIS
1	D	435	GLU
1	D	449	LYS
1	D	456	ASN
1	D	459	LEU
1	D	475	THR
1	D	484	LEU
1	D	490	GLU
1	D	500	ASP
1	D	549	ASP
1	D	587	VAL
1	D	626	VAL
1	D	644	VAL
1	D	647	GLU
1	D	653	ARG
1	D	681	LEU
1	D	682	GLN
1	D	694	VAL
1	D	748	THR
1	D	759	PHE
1	D	837	LEU
1	D	873	GLU
1	D	879	LEU

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	83	HIS
1	A	262	ASN
1	A	386	HIS
1	A	456	ASN
1	A	524	HIS
1	A	656	ASN
1	A	682	GLN
1	A	697	HIS
1	A	778	GLN
1	A	836	GLN
1	A	862	GLN
1	A	901	GLN
1	B	13	GLN
1	B	42	HIS
1	B	95	GLN
1	B	262	ASN
1	B	370	GLN
1	B	386	HIS
1	B	456	ASN
1	B	682	GLN
1	B	836	GLN
1	B	862	GLN
1	C	42	HIS
1	C	95	GLN
1	C	262	ASN
1	C	370	GLN
1	C	456	ASN
1	C	656	ASN
1	C	682	GLN
1	C	693	HIS
1	C	697	HIS
1	C	740	ASN
1	C	836	GLN
1	C	862	GLN
1	C	901	GLN
1	D	13	GLN
1	D	42	HIS
1	D	262	ASN
1	D	271	GLN
1	D	386	HIS
1	D	456	ASN
1	D	524	HIS
1	D	656	ASN

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Mol	Chain	Res	Type
1	D	682	GLN
1	D	693	HIS
1	D	697	HIS
1	D	836	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DTT	A	1923	-	7,7,7	0.55	0	4,8,8	0.73	0
2	DTT	C	1923	-	7,7,7	0.55	0	4,8,8	0.56	0
2	DTT	D	1923	-	7,7,7	0.56	0	4,8,8	0.31	0
2	DTT	B	1923	-	7,7,7	0.55	0	4,8,8	0.54	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
2	DTT	A	1923	-	-	3/8/8/8	-
2	DTT	C	1923	-	-	6/8/8/8	-
2	DTT	D	1923	-	-	2/8/8/8	-
2	DTT	B	1923	-	-	1/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1923	DTT	S1-C1-C2-O2
2	A	1923	DTT	C2-C3-C4-S4
2	A	1923	DTT	O3-C3-C4-S4
2	B	1923	DTT	S1-C1-C2-O2
2	C	1923	DTT	S1-C1-C2-O2
2	C	1923	DTT	S1-C1-C2-C3
2	C	1923	DTT	C1-C2-C3-O3
2	C	1923	DTT	C1-C2-C3-C4
2	C	1923	DTT	O2-C2-C3-O3
2	C	1923	DTT	O2-C2-C3-C4
2	D	1923	DTT	C2-C3-C4-S4
2	D	1923	DTT	O3-C3-C4-S4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1923	DTT	3	0
2	C	1923	DTT	1	0
2	B	1923	DTT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	889/923 (96%)	0.24	19 (2%) 63 55	53, 88, 126, 162	0
1	B	889/923 (96%)	0.29	25 (2%) 55 47	54, 88, 125, 163	0
1	C	889/923 (96%)	0.31	28 (3%) 51 44	54, 88, 124, 163	0
1	D	890/923 (96%)	0.19	19 (2%) 63 55	53, 88, 125, 162	0
All	All	3557/3692 (96%)	0.26	91 (2%) 57 49	53, 88, 125, 163	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	SER	4.4
1	B	42	HIS	3.4
1	C	143	LEU	3.2
1	B	126	VAL	3.2
1	C	116	ALA	3.1
1	A	126	VAL	3.1
1	D	548	LEU	3.0
1	A	452	ASP	3.0
1	D	57	VAL	3.0
1	D	492	VAL	3.0
1	D	473	VAL	2.9
1	C	126	VAL	2.9
1	A	680	LEU	2.8
1	A	595	LEU	2.8
1	B	815	PHE	2.7
1	B	185	MET	2.7
1	B	9	GLN	2.7
1	A	649	LEU	2.7
1	C	649	LEU	2.7
1	C	791	ALA	2.6
1	C	574	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	158	SER	2.6
1	D	153	GLU	2.6
1	B	595	LEU	2.5
1	D	680	LEU	2.5
1	C	578	THR	2.5
1	A	60	CYS	2.5
1	A	97	LEU	2.5
1	B	59	SER	2.5
1	A	473	VAL	2.5
1	C	747	ASP	2.4
1	C	60	CYS	2.4
1	D	572	LEU	2.4
1	D	453	PRO	2.4
1	B	673	VAL	2.4
1	D	182	SER	2.4
1	B	714	GLU	2.4
1	A	795	VAL	2.4
1	B	47	SER	2.4
1	B	458	THR	2.4
1	B	104	ILE	2.4
1	B	186	THR	2.3
1	C	453	PRO	2.3
1	B	454	GLU	2.3
1	B	536	GLN	2.3
1	C	595	LEU	2.3
1	C	642	TRP	2.3
1	C	656	ASN	2.3
1	A	57	VAL	2.3
1	B	137	VAL	2.3
1	D	626	VAL	2.3
1	C	680	LEU	2.3
1	D	449	LYS	2.3
1	D	280	TYR	2.3
1	B	625	ILE	2.2
1	C	815	PHE	2.2
1	B	97	LEU	2.2
1	B	615	LEU	2.2
1	C	211	LEU	2.2
1	B	278	THR	2.2
1	A	420	PHE	2.2
1	A	27	LYS	2.2
1	A	469	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	108	LEU	2.2
1	C	710	GLU	2.2
1	D	112	ILE	2.2
1	D	47	SER	2.2
1	C	311	VAL	2.2
1	C	185	MET	2.2
1	B	548	LEU	2.1
1	D	173	LEU	2.1
1	D	544	ILE	2.1
1	B	225	LEU	2.1
1	A	101	SER	2.1
1	B	60	CYS	2.1
1	C	171	GLU	2.1
1	C	189	GLU	2.1
1	A	143	LEU	2.1
1	C	144	LEU	2.1
1	C	17	ALA	2.1
1	C	207	SER	2.1
1	B	691	VAL	2.1
1	A	144	LEU	2.1
1	D	186	THR	2.1
1	C	570	ALA	2.1
1	C	651	LYS	2.0
1	C	360	VAL	2.0
1	A	100	LEU	2.0
1	A	735	LEU	2.0
1	D	85	SER	2.0
1	D	154	VAL	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($\text{\AA}^2$)	Q<0.9
2	DTT	C	1923	8/8	0.83	0.13	85,111,121,143	0
2	DTT	B	1923	8/8	0.87	0.12	92,104,134,144	0
2	DTT	D	1923	8/8	0.88	0.12	79,94,108,114	0
2	DTT	A	1923	8/8	0.89	0.11	72,99,109,126	0

6.5 Other polymers [i](#)

There are no such residues in this entry.