Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:26 PM BST

PDB ID	:	4C0P
Title	:	Unliganded Transportin 3
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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 following versions of software and data (see references ⓘ) were used in the production of this report:

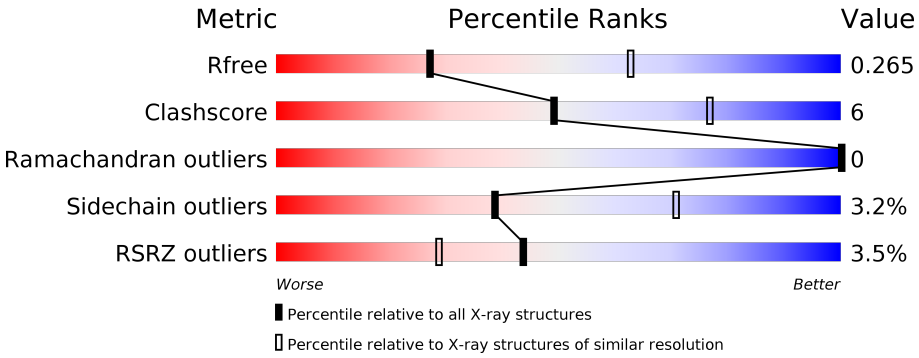
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	923	4% 79% 16%
1	B	923	3% 79% 16%
1	C	923	4% 80% 16%
1	D	923	3% 79% 16%

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.

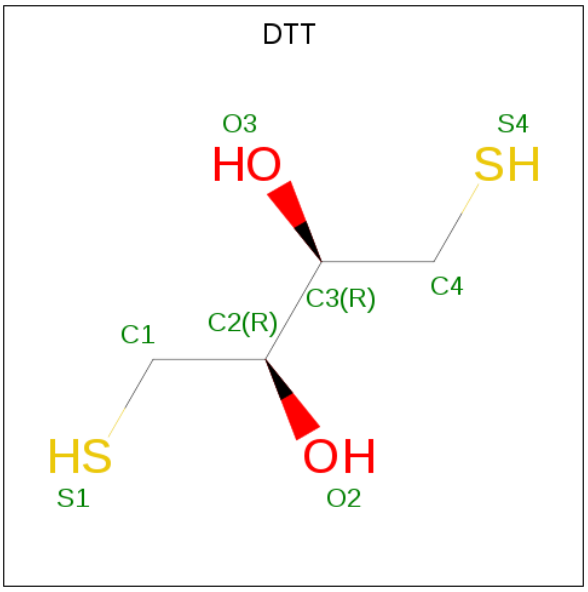
- Molecule 1 is a protein called TRANSPORTIN-3.

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 (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



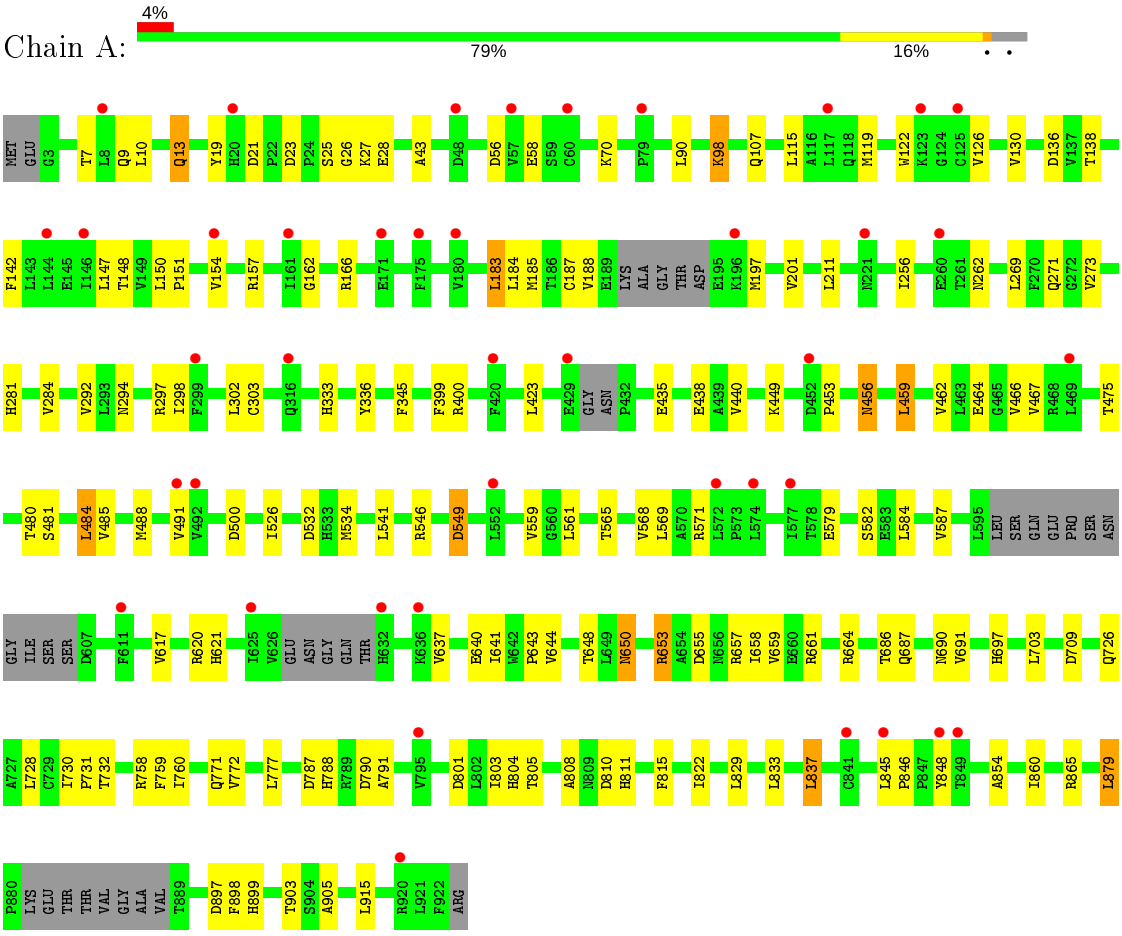
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 8 4 2 2	0	0
2	B	1	Total C O S 8 4 2 2	0	0
2	C	1	Total C O S 8 4 2 2	0	0
2	D	1	Total C O S 8 4 2 2	0	0

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.

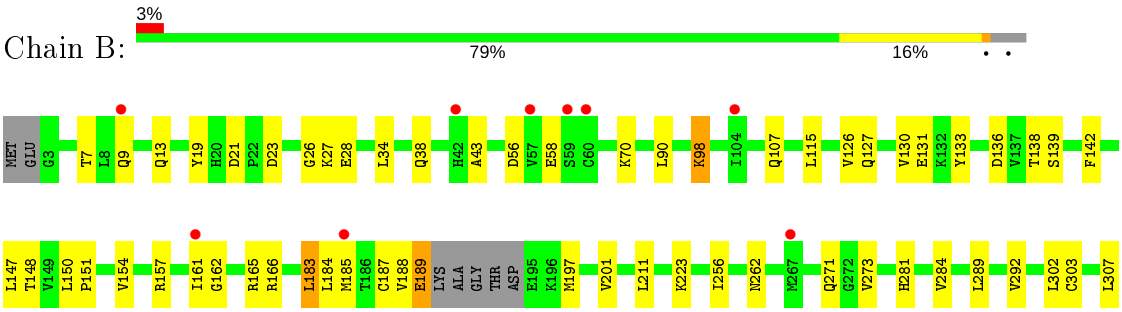
- Molecule 1: TRANSPORTIN-3

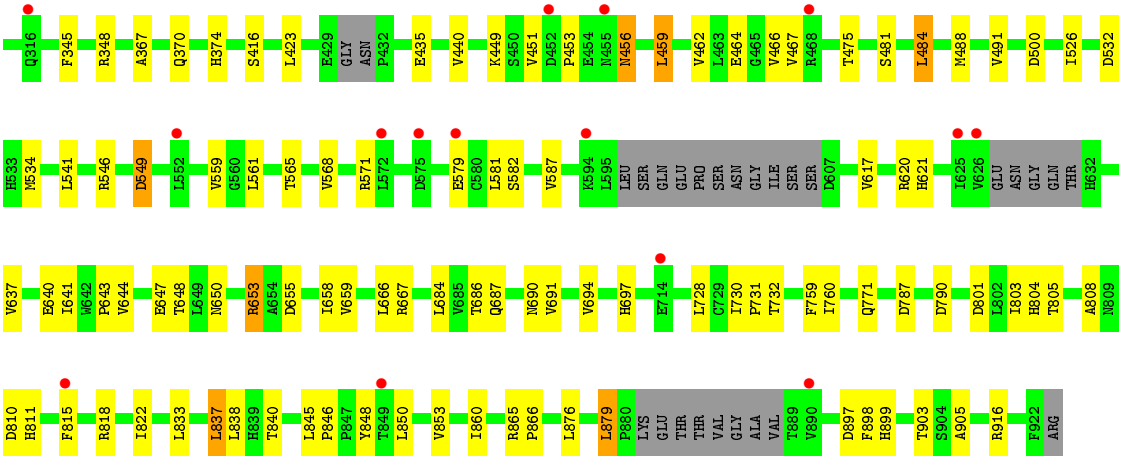
Chain A:



- Molecule 1: TRANSPORTIN-3

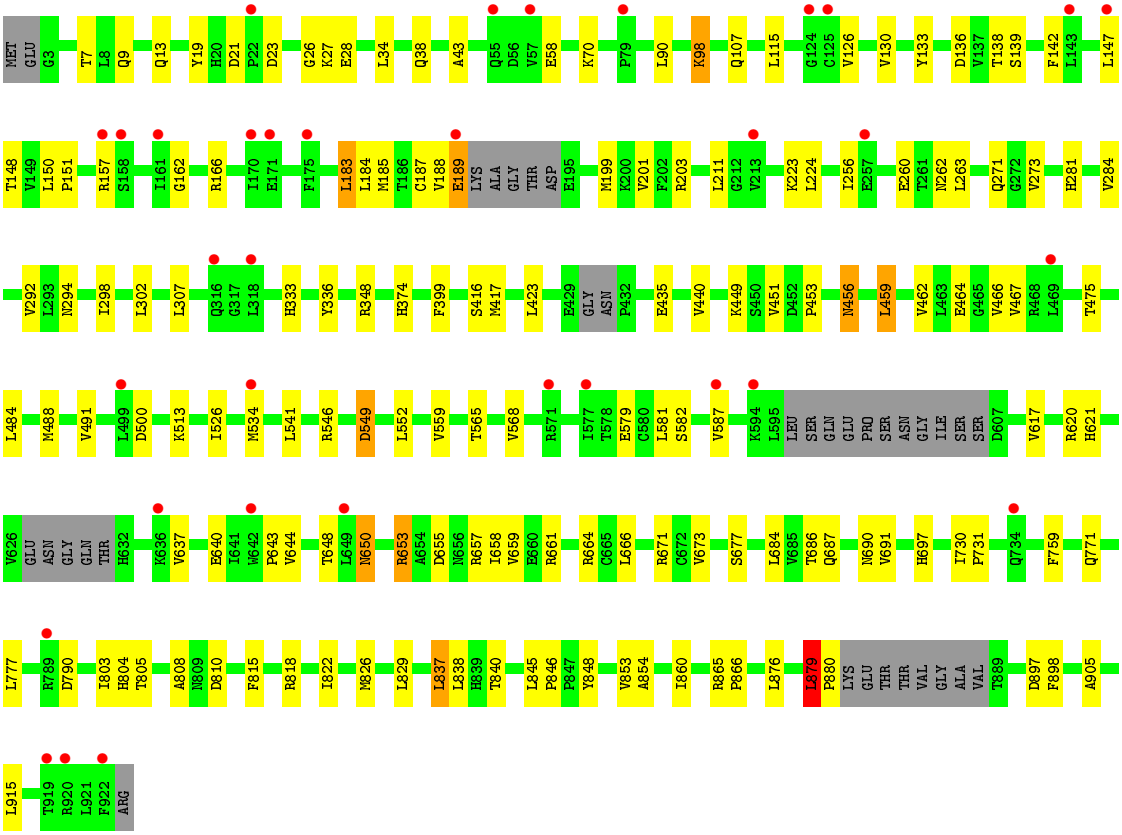
Chain B:





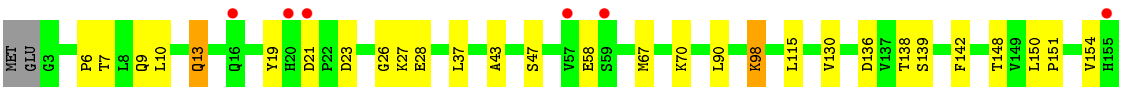
• Molecule 1: TRANSPORTIN-3

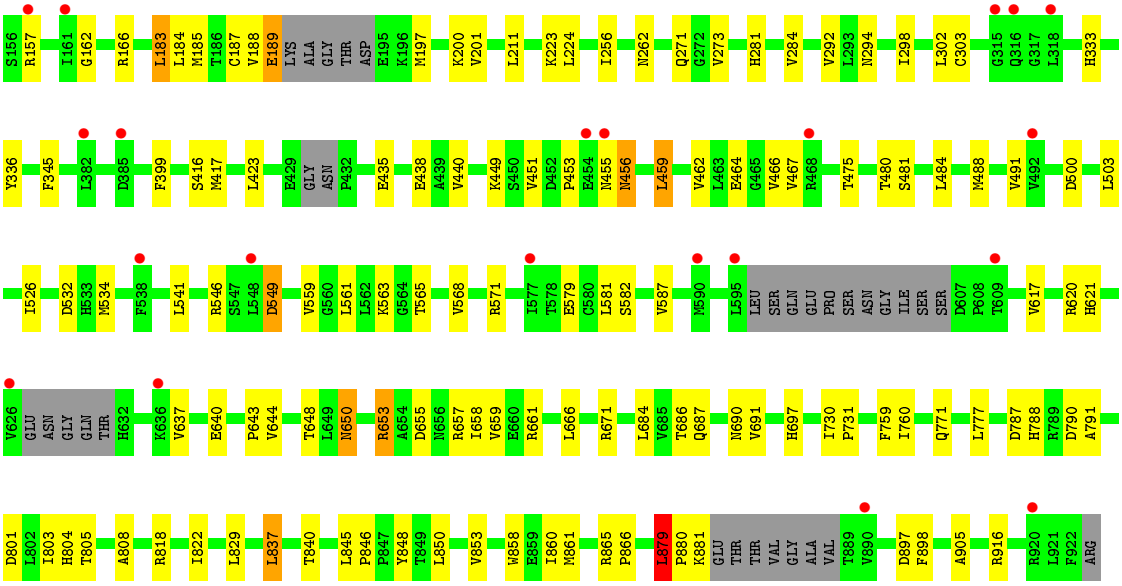
Chain C:



• Molecule 1: TRANSPORTIN-3

Chain D:




S156 R157 I161 G162 R166 L183 L184 M185 T186 C187 V188 E189 LYS ALA GLY THR ASP E195 K196 M197 K200 V201 L211 K223 L224 I256 N262 Q271 G272 V273 H281 V284 V292 L293 N294 I298 L302 C303 G315 Q316 G317 L318 H333
Y336 F345 L382 D386 F399 S416 M417 L423 E429 GLY ASN P432 E435 E438 A439 V440 K449 S450 V451 D452 P453 E454 N455 N456 L459 V462 L463 E464 G465 V466 V467 R468 T475 T480 S481 L484 M488 V491 V492 D500 L503
I526 D532 H533 M534 F538 L541 R546 S547 L548 D549 V559 G560 L561 L562 K563 G564 T565 V568 R571 I577 T578 E579 C580 L581 S582 V587 M590 L595 LEU SER GLN GLU PRO SER ASN GLY ILE SER SER D607 P608 T609 V617 R620 H621
V626 GLU ASN GLY GLN THR H632 K636 V637 E640 P643 V644 T648 L649 N650 R653 A654 D655 M656 R657 I658 V659 E660 R661 L666 R671 L684 V685 T686 Q687 N690 V691 H697 I730 P731 F759 I760 Q771 L777 D787 H788 R789 D790 A791
D801 L802 I803 H804 T805 A808 R818 I822 L829 L837 T840 L845 P846 P847 Y848 T849 L850 V853 W858 E859 I860 M861 R865 P866 L879 P880 K881 GLU THR THR VAL GLY ALA VAL T889 V890 D897 F898 A905 R916 R920 L921 F922 ARG

4 Data and refinement statistics (i)

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 39.80 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.1 (38.17-2.95) 98.5 (39.80-2.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.236 , 0.266 0.236 , 0.265	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 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[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: 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	0.23	0/7203	0.42	1/9779 (0.0%)
1	B	0.23	0/7203	0.42	1/9779 (0.0%)
1	C	0.23	0/7203	0.42	1/9779 (0.0%)
1	D	0.23	0/7212	0.42	1/9790 (0.0%)
All	All	0.23	0/28821	0.42	4/39127 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	879	LEU	CA-CB-CG	5.27	127.42	115.30
1	D	879	LEU	CA-CB-CG	5.25	127.39	115.30
1	C	879	LEU	CA-CB-CG	5.16	127.16	115.30
1	B	879	LEU	CA-CB-CG	5.13	127.10	115.30

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	7063	0	7102	86	0
1	B	7063	0	7102	85	0
1	C	7063	0	7102	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	7072	0	7115	87	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	336	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 (336) 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:D:21:ASP:O	1:D:27:LYS:NZ	2.09	0.85
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	0.82
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: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: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:184:LEU:HG	1:B:201:VAL:HG13	1.75	0.68
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: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:B:549:ASP:N	1:B:549:ASP:OD1	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:549:ASP:OD1	2.33	0.61
1:D:549:ASP:N	1:D:549:ASP:OD1	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: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
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:D:526:ILE:HG22	1:D:534:MET:HE3	1.85	0.56
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:A:526:ILE:HG22	1:A:534:MET:HE3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:526:ILE:HG22	1:B:534:MET:HE3	1.90	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: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
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:C:526:ILE:HG22	1:C:534:MET:HE3	1.92	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: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:162:GLY:O	1:B:166:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:803:ILE:HD11	1:B:833:LEU:HD21	1.93	0.50
1:B:98:LYS:HG3	1:B:142:PHE:HD2	1.77	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: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: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:A:559:VAL:HG13	1:A:617:VAL:HG21	1.94	0.49
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: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:N	1:B:771:GLN:OE1	2.45	0.48
1:B:837:LEU:HG	1:B:853:VAL:HG13	1.95	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:D:150:LEU:HB3	1:D:151:PRO:HD3	1.96	0.47
1:D:423:LEU:HB3	1:D:440:VAL:HG13	1.95	0.47
1:D:416:SER:HB2	1:D:451:VAL:HG22	1.95	0.47
1:D:657:ARG:O	1:D:661:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:MET:HG3	1:D:197:MET:O	2.15	0.47
1:C:846:PRO:HB2	1:C:848:TYR:CD1	2.50	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: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
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:O	1:B:197:MET:HG3	2.15	0.46
1:D:805:THR:HB	1:D:822:ILE:HD11	1.97	0.46
1:D:803:ILE:HD13	1:D:860:ILE:HG12	1.96	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: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:B:728:LEU:O	1:B:732:THR:OG1	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:728:LEU:O	1:A:732:THR:OG1	2.22	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
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:703:LEU:HB2	2:A:1923:DTT:S1	2.57	0.44
1:A:644:VAL:O	1:A:648:THR:OG1	2.28	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: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:C:417:MET:HE3	1:C:456:ASN:HB2	2.01	0.43
1:D:644:VAL:O	1:D:648:THR:OG1	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:858:TRP:HA	1:D:861:MET:HE3	2.00	0.43
1:B:837:LEU:HA	1:B:837:LEU:HD12	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
1:D:7:THR:HG22	1:D:9:GLN:H	1.83	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: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: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:459:LEU:H	1:B:459:LEU:HG	1.67	0.42
1:B:56:ASP:HB3	1:B:58:GLU:OE1	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:563:LYS:HE3	1:D:621:HIS:CD2	2.56	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:417:MET:HE3	1:D:456:ASN:HB2	2.03	0.41
1:D:455:ASN:N	1:D:455:ASN:OD1	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:B:899:HIS:CE1	1:B:903:THR:HG21	2.55	0.41
1:D:579:GLU:O	1:D:582:SER:OG	2.36	0.41
1:A:569:LEU:HD22	1:A:584:LEU:HD13	2.03	0.41
1:D:224:LEU:HA	1:D:224:LEU:HD12	1.83	0.41
1:D:503:LEU:HD11	1:D:534:MET:SD	2.61	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:B:644:VAL:O	1:B:648:THR:OG1	2.24	0.40
1:C:840:THR:HG23	1:C:845:LEU:HG	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3509/3692 (95%)	3389 (97%)	120 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	793/820 (97%)	768 (97%)	25 (3%)	39 71
1	B	793/820 (97%)	766 (97%)	27 (3%)	37 69
1	C	793/820 (97%)	767 (97%)	26 (3%)	38 70
1	D	794/820 (97%)	769 (97%)	25 (3%)	40 71
All	All	3173/3280 (97%)	3070 (97%)	103 (3%)	39 71

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	25	SER
1	A	28	GLU
1	A	98	LYS
1	A	107	GLN
1	A	157	ARG
1	A	183	LEU
1	A	187	CYS
1	A	271	GLN
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	500	ASP
1	A	546	ARG

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Mol	Chain	Res	Type
1	A	549	ASP
1	A	587	VAL
1	A	650	ASN
1	A	653	ARG
1	A	759	PHE
1	A	790	ASP
1	A	837	LEU
1	A	879	LEU
1	B	13	GLN
1	B	28	GLU
1	B	98	LYS
1	B	107	GLN
1	B	157	ARG
1	B	183	LEU
1	B	187	CYS
1	B	189	GLU
1	B	271	GLN
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	500	ASP
1	B	546	ARG
1	B	549	ASP
1	B	587	VAL
1	B	647	GLU
1	B	650	ASN
1	B	653	ARG
1	B	759	PHE
1	B	790	ASP
1	B	837	LEU
1	B	879	LEU
1	C	13	GLN
1	C	28	GLU
1	C	98	LYS
1	C	107	GLN
1	C	157	ARG
1	C	183	LEU
1	C	187	CYS

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Mol	Chain	Res	Type
1	C	189	GLU
1	C	271	GLN
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	500	ASP
1	C	546	ARG
1	C	549	ASP
1	C	587	VAL
1	C	650	ASN
1	C	653	ARG
1	C	759	PHE
1	C	790	ASP
1	C	837	LEU
1	C	879	LEU
1	D	13	GLN
1	D	28	GLU
1	D	98	LYS
1	D	157	ARG
1	D	183	LEU
1	D	187	CYS
1	D	189	GLU
1	D	271	GLN
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	500	ASP
1	D	546	ARG
1	D	549	ASP
1	D	587	VAL
1	D	650	ASN
1	D	653	ARG
1	D	759	PHE
1	D	790	ASP
1	D	837	LEU

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Mol	Chain	Res	Type
1	D	879	LEU
1	D	881	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	456	ASN
1	A	738	GLN
1	B	456	ASN
1	B	738	GLN
1	C	456	ASN
1	D	456	ASN
1	D	738	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

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	D	1923	-	7,7,7	0.55	0	4,8,8	0.32	0
2	DTT	C	1923	-	7,7,7	0.55	0	4,8,8	0.55	0
2	DTT	B	1923	-	7,7,7	0.55	0	4,8,8	0.53	0
2	DTT	A	1923	-	7,7,7	0.55	0	4,8,8	0.71	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	D	1923	-	-	2/8/8/8	-
2	DTT	C	1923	-	-	6/8/8/8	-
2	DTT	B	1923	-	-	1/8/8/8	-
2	DTT	A	1923	-	-	3/8/8/8	-

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	D	1923	DTT	C2-C3-C4-S4
2	D	1923	DTT	O3-C3-C4-S4
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	B	1923	DTT	S1-C1-C2-O2
2	A	1923	DTT	S1-C1-C2-O2
2	A	1923	DTT	C2-C3-C4-S4
2	A	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	C	1923	DTT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1923	DTT	1	0
2	A	1923	DTT	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	889/923 (96%)	0.34	41 (4%)	32	20	53, 88, 126, 162	0
1	B	889/923 (96%)	0.31	24 (2%)	54	38	54, 88, 125, 163	0
1	C	889/923 (96%)	0.37	34 (3%)	40	26	54, 88, 124, 163	0
1	D	890/923 (96%)	0.30	27 (3%)	50	34	53, 88, 125, 162	0
All	All	3557/3692 (96%)	0.33	126 (3%)	44	29	53, 88, 125, 163	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	57	VAL	5.3
1	A	452	ASP	4.7
1	B	468	ARG	4.4
1	B	594	LYS	4.2
1	B	626	VAL	4.1
1	D	548	LEU	4.0
1	C	22	PRO	4.0
1	B	42	HIS	3.9
1	A	849	THR	3.7
1	C	171	GLU	3.6
1	A	795	VAL	3.6
1	A	636	LYS	3.6
1	D	455	ASN	3.5
1	A	221	ASN	3.5
1	B	161	ILE	3.5
1	D	626	VAL	3.5
1	B	714	GLU	3.4
1	A	171	GLU	3.4
1	B	455	ASN	3.3
1	B	849	THR	3.3
1	C	161	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	196	LYS	3.2
1	C	147	LEU	3.2
1	D	492	VAL	3.1
1	D	636	LYS	3.1
1	C	499	LEU	3.1
1	D	59	SER	3.0
1	A	260	GLU	3.0
1	B	59	SER	3.0
1	C	158	SER	2.9
1	D	385	ASP	2.9
1	D	577	ILE	2.9
1	B	890	VAL	2.9
1	B	575	ASP	2.9
1	A	625	ILE	2.8
1	D	590	MET	2.8
1	C	157	ARG	2.8
1	C	175	PHE	2.8
1	A	79	PRO	2.8
1	D	468	ARG	2.8
1	A	848	TYR	2.8
1	C	316	GLN	2.8
1	C	189	GLU	2.8
1	C	257	GLU	2.8
1	A	8	LEU	2.8
1	B	185	MET	2.7
1	D	382	LEU	2.7
1	C	534	MET	2.7
1	B	57	VAL	2.7
1	B	579	GLU	2.7
1	A	161	ILE	2.6
1	A	845	LEU	2.6
1	C	55	GLN	2.6
1	C	571	ARG	2.6
1	C	920	ARG	2.6
1	A	920	ARG	2.6
1	A	577	ILE	2.6
1	A	469	LEU	2.6
1	A	574	LEU	2.6
1	D	21	ASP	2.6
1	C	79	PRO	2.6
1	A	420	PHE	2.6
1	C	642	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	552	LEU	2.5
1	A	57	VAL	2.5
1	A	180	VAL	2.5
1	D	16	GLN	2.5
1	C	170	ILE	2.5
1	D	595	LEU	2.4
1	B	625	ILE	2.4
1	A	611	PHE	2.4
1	B	267	MET	2.4
1	C	789	ARG	2.4
1	C	125	CYS	2.4
1	B	815	PHE	2.3
1	A	60	CYS	2.3
1	A	48	ASP	2.3
1	D	315	GLY	2.3
1	A	117	LEU	2.3
1	A	299	PHE	2.3
1	D	20	HIS	2.3
1	D	161	ILE	2.3
1	A	20	HIS	2.2
1	B	452	ASP	2.2
1	B	572	LEU	2.2
1	C	919	THR	2.2
1	A	125	CYS	2.2
1	A	492	VAL	2.2
1	C	57	VAL	2.2
1	D	920	ARG	2.2
1	C	213	VAL	2.2
1	D	609	THR	2.2
1	C	636	LYS	2.2
1	A	429	GLU	2.2
1	B	104	ILE	2.2
1	B	9	GLN	2.2
1	A	572	LEU	2.2
1	C	318	LEU	2.2
1	C	649	LEU	2.2
1	C	577	ILE	2.2
1	B	60	CYS	2.2
1	D	890	VAL	2.2
1	C	143	LEU	2.1
1	B	316	GLN	2.1
1	D	316	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	594	LYS	2.1
1	D	318	LEU	2.1
1	A	316	GLN	2.1
1	A	175	PHE	2.1
1	C	922	PHE	2.1
1	C	587	VAL	2.1
1	D	157	ARG	2.1
1	C	124	GLY	2.1
1	A	491	VAL	2.1
1	D	538	PHE	2.1
1	A	144	LEU	2.1
1	C	469	LEU	2.1
1	A	146	ILE	2.1
1	A	123	LYS	2.1
1	A	841	CYS	2.0
1	A	154	VAL	2.0
1	A	552	LEU	2.0
1	C	734	GLN	2.0
1	D	155	HIS	2.0
1	A	632	HIS	2.0
1	D	454	GLU	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
2	DTT	C	1923	8/8	0.77	0.33	85,111,121,143	0
2	DTT	A	1923	8/8	0.84	0.28	72,99,109,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DTT	D	1923	8/8	0.87	0.24	79,94,108,114	0
2	DTT	B	1923	8/8	0.88	0.23	92,104,134,144	0

6.5 Other polymers (i)

There are no such residues in this entry.