Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:19 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

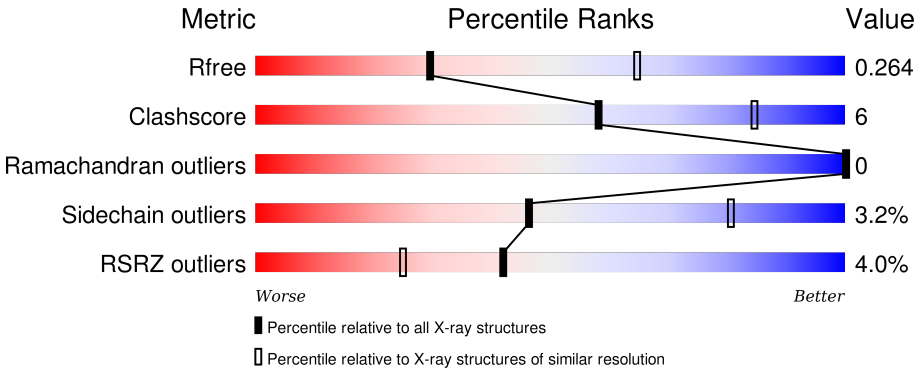
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (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. 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	5% 79% 16%
1	B	923	3% 79% 16%
1	C	923	4% 80% 16%
1	D	923	3% 79% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DTT	C	1923	-	-	-	X

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.

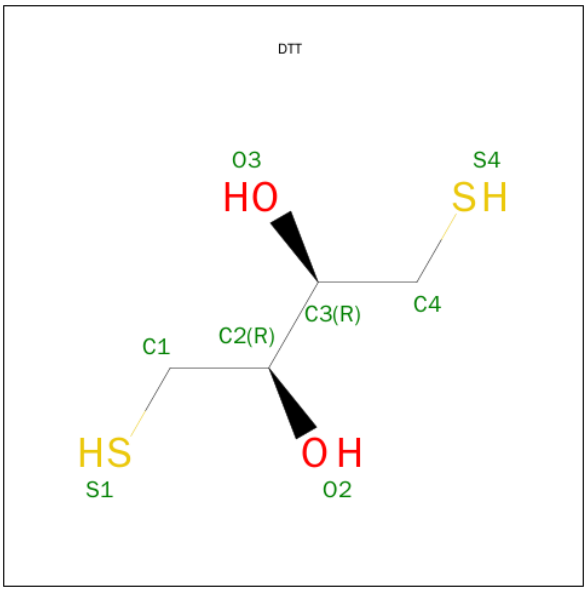
- Molecule 1 is a protein called TRANSPORTIN-3.

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: $C_4H_{10}O_2S_2$).



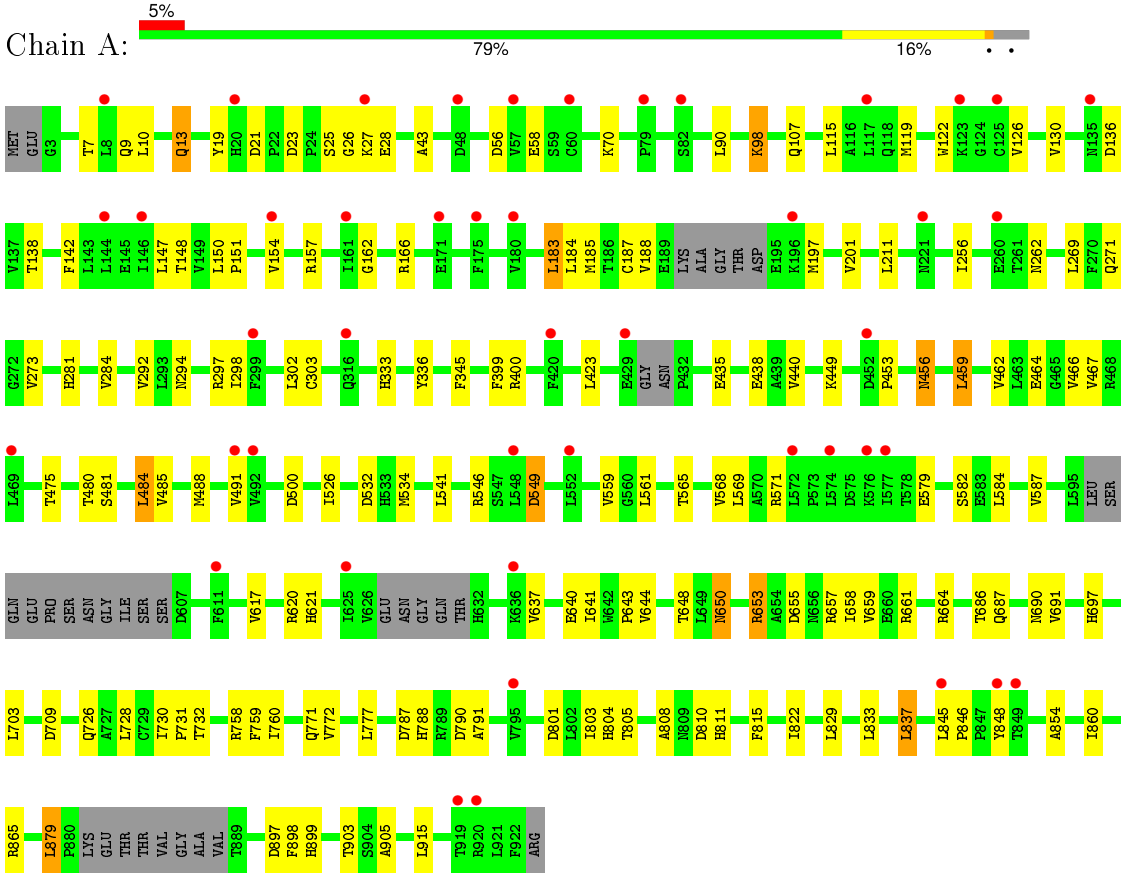
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 8 4 2 2	0	0
2	B	1	Total C O S 8 4 2 2	0	0
2	C	1	Total C O S 8 4 2 2	0	0
2	D	1	Total C O S 8 4 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

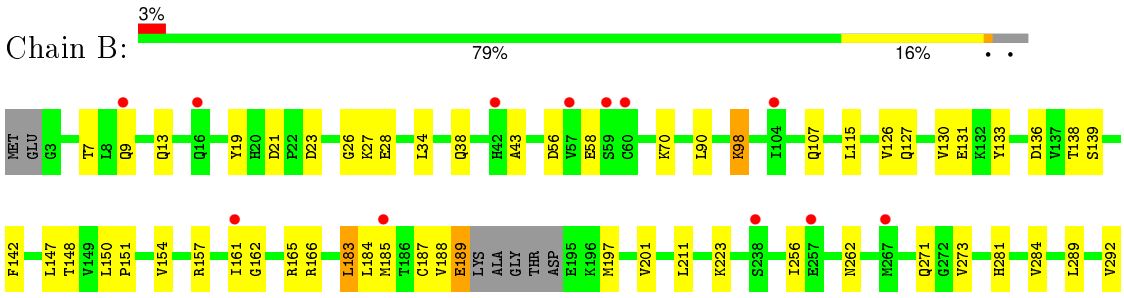
- Molecule 1: TRANSPORTIN-3

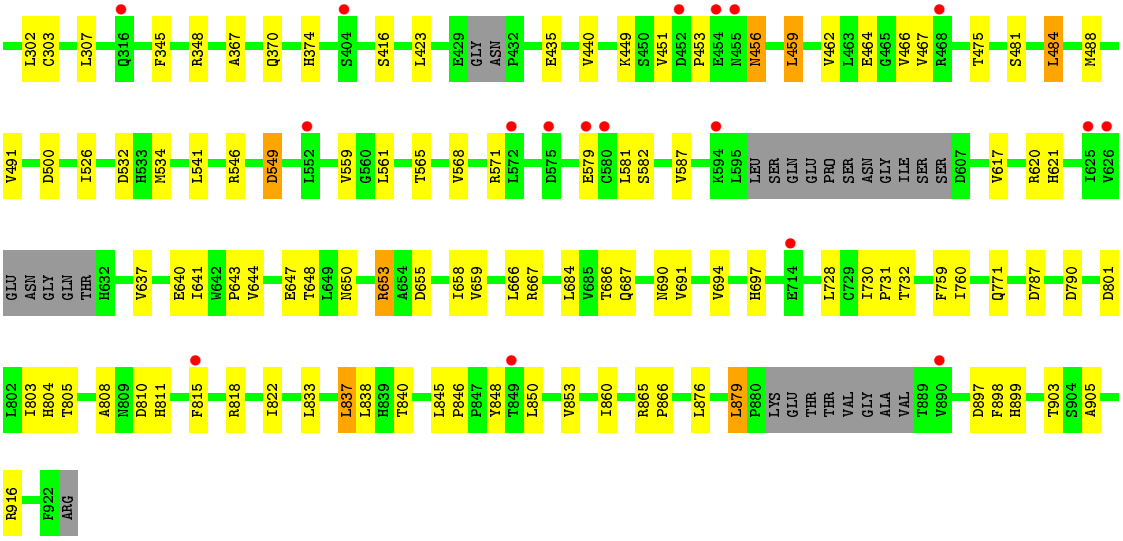
Chain A:



- Molecule 1: TRANSPORTIN-3

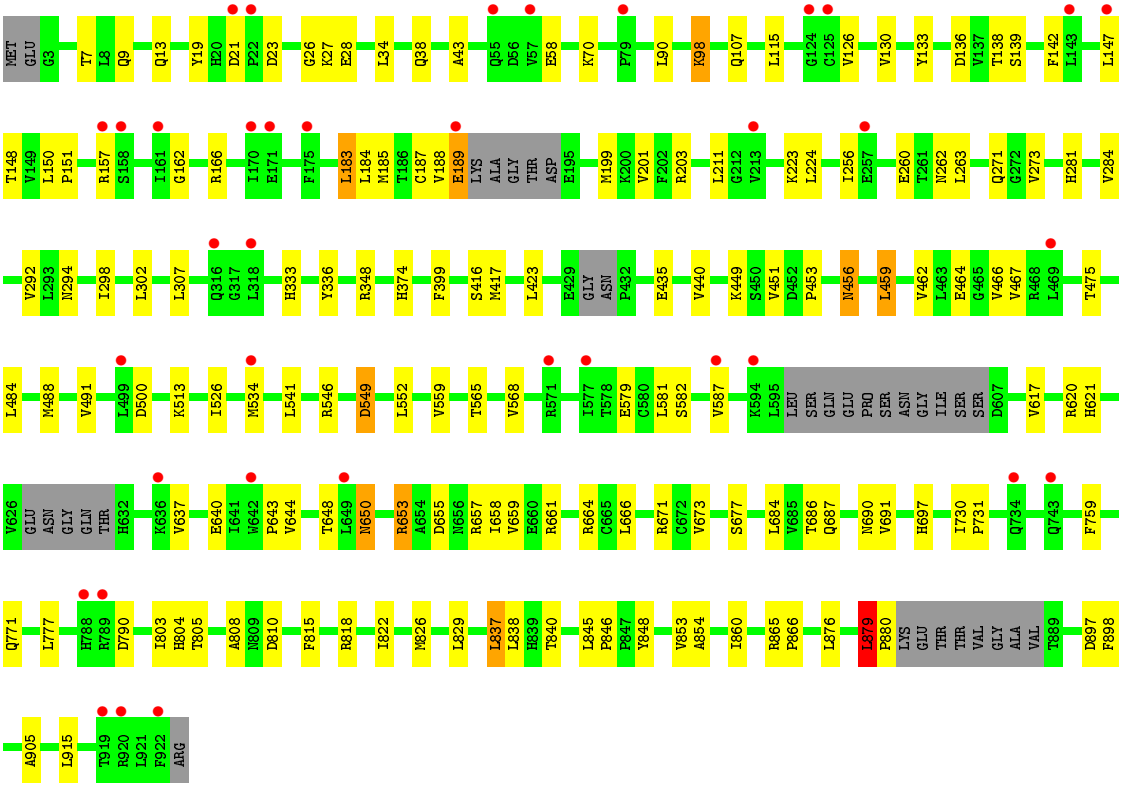
Chain B:





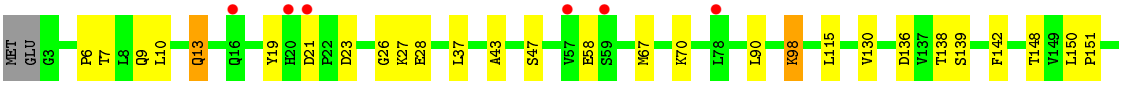
• Molecule 1: TRANSPORTIN-3

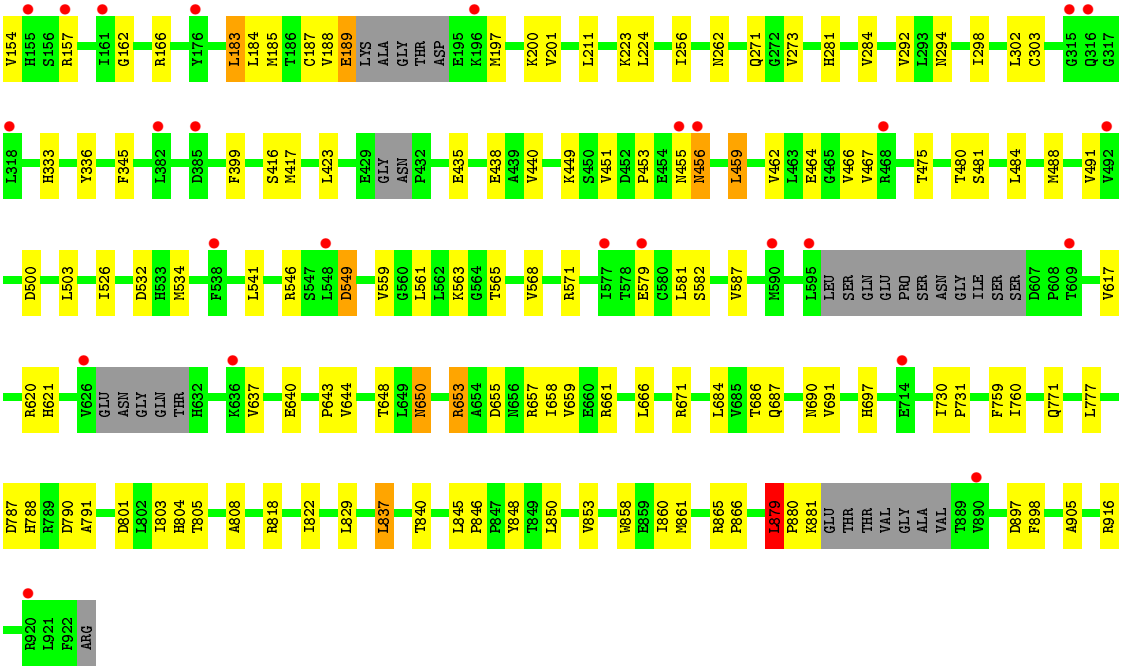
Chain C:



• Molecule 1: TRANSPORTIN-3

Chain D:




V154 H155 S156 R157 I161 G162 R166 Y176 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 D385 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 N656 R657 I658 V659 E660 R661 L666 R671 L684 V685 T686 Q687 N690 V691 H697 E714 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) 97.0 (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 0.233 , 0.264	Depositor DCC
R_{free} test set	4857 reflections (5.05%)	DCC
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 , 56.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 96209 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:459:LEU:HB2	1:B:491:VAL:HG21	1.78	0.66
1:B:273:VAL:HG11	1:B:302:LEU:HD13	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:C:865:ARG:NH2	1:C:905:ALA:O	2.34	0.60
1:A:400:ARG:NH2	1:A:438:GLU:OE2	2.33	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:D:532:ASP:OD1	1:D:571:ARG:NH1	2.38	0.57
1:C:189:GLU:OE2	1:C:223:LYS:NZ	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:D:534:MET:HG2	1:D:568:VAL:HG11	1.87	0.56
1:A:687:GLN:O	1:A:691:VAL:HG12	2.06	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:C:686:THR:O	1:C:690:ASN:ND2	2.39	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: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:C:136:ASP:O	1:C:138:THR:N	2.39	0.53
1:A:659:VAL:HG11	1:A:697:HIS:CD2	2.44	0.53
1:B:534:MET:HG2	1:B:568:VAL:HG11	1.90	0.52
1:B:189:GLU:OE2	1:B:223:LYS:NZ	2.40	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:664:ARG:NH1	2:A:1923:DTT:H42	2.26	0.51
1:A:650:ASN:O	1:A:653:ARG:HD2	2.11	0.51
1:A:423:LEU:HB3	1:A:440:VAL:HG13	1.93	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:98:LYS:HG3	1:B:142:PHE:HD2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N	1:D:771:GLN:OE1	2.45	0.49
1:C:653:ARG:HB2	1:C:691:VAL:HG23	1.94	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: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:B:805:THR:HB	1:B:822:ILE:HD11	1.94	0.48
1:A:98:LYS:HG3	1:A:142:PHE:HD2	1.78	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:804:HIS:NE2	1:D:808:ALA:HB2	2.28	0.48
1:D:292:VAL:HG21	1:D:333:HIS:CD2	2.49	0.48
1:D:650:ASN:O	1:D:653:ARG:HD2	2.14	0.48
1:A:846:PRO:HB2	1:A:848:TYR:CD1	2.48	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: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

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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:D:438:GLU:OE2	1:D:480:THR:HG21	2.15	0.47
1:C:846:PRO:HB2	1:C:848:TYR:CD1	2.50	0.47
1:B:805:THR:O	1:B:818:ARG:NH1	2.45	0.47
1:B:846:PRO:HB2	1:B:848:TYR:CD1	2.50	0.47
1:B:579:GLU:O	1:B:582:SER:OG	2.30	0.47
1:A:771:GLN:N	1:A:771:GLN:OE1	2.44	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:C:148:THR:O	1:C:151:PRO:HD2	2.15	0.46
1:B:803:ILE:HD13	1:B:860:ILE:HG12	1.97	0.46
1:C:771:GLN:OE1	1:C:771:GLN:N	2.44	0.46
1:D:803:ILE:HD13	1:D:860:ILE:HG12	1.96	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: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:803:ILE:HD11	1:A:833:LEU:HD21	1.97	0.46
1:C:423:LEU:HB3	1:C:440:VAL:HG13	1.97	0.46
1:C:805:THR:HG22	1:C:818:ARG:HD2	1.98	0.46
1:B:7:THR:HG22	1:B:9:GLN:H	1.79	0.46
1:C:730:ILE:HB	1:C:731:PRO:HD3	1.98	0.46
1:A:899:HIS:CE1	1:A:903:THR:HG21	2.51	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:B:289:LEU:HA	1:B:292:VAL:HG12	1.98	0.46
1:A:126:VAL:HG13	1:A:147:LEU:HD11	1.98	0.46
1:C:810:ASP:HA	1:C:815:PHE:CG	2.51	0.45
1:A:777:LEU:HD23	1:A:829:LEU:HD12	1.98	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:C:488:MET:O	1:C:491:VAL:HG12	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: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:B:151:PRO:O	1:B:154:VAL:HG12	2.17	0.45
1:A:162:GLY:O	1:A:166:ARG:NH1	2.49	0.45
1:C:464:GLU:HA	1:C:467:VAL:HG22	1.97	0.45
1:A:728:LEU:O	1:A:732:THR:OG1	2.22	0.45
1:C:559:VAL:HG13	1:C:617:VAL:HG21	1.99	0.45
1:B:464:GLU:HA	1:B:467:VAL:HG22	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:D:464:GLU:HA	1:D:467:VAL:HG22	1.99	0.45
1:C:336:TYR:HB2	1:C:399:PHE:CZ	2.51	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:B:484:LEU:O	1:B:488:MET:HG3	2.17	0.45
1:A:464:GLU:HA	1:A:467:VAL:HG22	1.99	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:C:805:THR:O	1:C:818:ARG:NH1	2.48	0.44
1:A:644:VAL:O	1:A:648:THR:OG1	2.28	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:D:760:ILE:HG21	1:D:801:ASP:HB3	2.00	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:C:804:HIS:NE2	1:C:808:ALA:HB2	2.33	0.44
1:C:185:MET:O	1:C:188:VAL:HG22	2.18	0.44
1:D:655:ASP:OD1	1:D:658:ILE:HG12	2.18	0.44
1:C:879:LEU:HA	1:C:880:PRO:HD3	1.87	0.43
1:C:838:LEU:HD21	1:C:876:LEU:HD23	2.00	0.43
1:C:417:MET:HE3	1:C:456:ASN:HB2	2.01	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: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:B:488:MET:O	1:B:491:VAL:HG12	2.18	0.43
1:A:484:LEU:O	1:A:488:MET:HG3	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: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:D:777:LEU:HD23	1:D:829:LEU:HD12	1.99	0.43
1:B:811:HIS:HB3	1:C:671:ARG:NH2	2.33	0.43
1:A:657:ARG:O	1:A:661:ARG:HG2	2.18	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:D:336:TYR:HB2	1:D:399:PHE:CZ	2.54	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: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:D:563:LYS:HE3	1:D:621:HIS:NE2	2.34	0.42
1:C:162:GLY:O	1:C:166:ARG:NH1	2.52	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:A:462:VAL:O	1:A:466:VAL:HG23	2.20	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:C:462:VAL:O	1:C:466:VAL:HG23	2.20	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:A:561:LEU:O	1:A:565:THR:HG23	2.20	0.42
1:B:760:ILE:HG21	1:B:801:ASP:HB3	2.02	0.42
1:A:730:ILE:HB	1:A:731:PRO:HD3	2.01	0.42
1:D:488:MET:O	1:D:491:VAL:HG12	2.19	0.42
1:C:307:LEU:HD13	1:C:348:ARG:NH1	2.35	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:D:303:CYS:HB3	1:D:345:PHE:CE1	2.55	0.42
1:C:657:ARG:O	1:C:661:ARG:HG2	2.20	0.42
1:B:637:VAL:O	1:B:641:ILE:HG13	2.20	0.41
1:D:787:ASP:HA	1:D:845:LEU:HD22	2.01	0.41
1:B:840:THR:HG23	1:B:845:LEU:HG	2.02	0.41
1:A:481:SER:O	1:A:485:VAL:HG23	2.20	0.41
1:D:653:ARG:HB2	1:D:691:VAL:HG23	2.02	0.41
1:D:200:LYS:HA	1:D:200:LYS:HD3	1.82	0.41
1:B:653:ARG:NH2	1:B:694:VAL:HG11	2.35	0.41
1:B:416:SER:HB2	1:B:451:VAL:HG22	2.01	0.41
1:A:637:VAL:O	1:A:641:ILE:HG13	2.20	0.41
1:D:865:ARG:N	1:D:866:PRO:HD2	2.36	0.41
1:A:256:ILE:HD11	1:A:269:LEU:HD12	2.02	0.41
1:D:804:HIS:CD2	1:D:808:ALA:HB2	2.56	0.41
1:A:294:ASN:O	1:A:298:ILE:HG13	2.20	0.41
1:C:260:GLU:HA	1:C:263:LEU:HG	2.02	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: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:D:417:MET:HE3	1:D:456:ASN:HB2	2.03	0.41
1:C:810:ASP:HA	1:C:815:PHE:CD1	2.56	0.41
1:D:455:ASN:N	1:D:455:ASN:OD1	2.54	0.41
1:C:292:VAL:HG21	1:C:333:HIS:CD2	2.56	0.41
1:C:822:ILE:HG23	1:C:826:MET:HG3	2.02	0.41
1:C:199:MET:O	1:C:203:ARG:HG3	2.21	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:B:899:HIS:CE1	1:B:903:THR:HG21	2.55	0.41
1:D:788:HIS:HB3	1:D:791:ALA:HB3	2.02	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: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:788:HIS:HB3	1:A:791:ALA:HB3	2.01	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: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
1:B:303:CYS:HB3	1:B:345:PHE:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:561:LEU:O	1:D:565:THR:HG23	2.20	0.40
1:A:294:ASN:OD1	1:A:297:ARG:NH1	2.54	0.40
1:D:466:VAL:HG13	1:D:481:SER:HB2	2.02	0.40
1:B:161:ILE:HG13	1:B:165:ARG:HG2	2.04	0.40
1:A:119:MET:SD	1:A:122:TRP:HB2	2.62	0.40
1:A:787:ASP:HA	1:A:845:LEU:HD22	2.04	0.40
1:B:561:LEU:HD12	1:B:561:LEU:HA	1.82	0.40
1:A:760:ILE:HD13	1:A:760:ILE:HA	1.89	0.40
1:D:462:VAL:O	1:D:466:VAL:HG23	2.21	0.40
1:A:640:GLU:O	1:A:643:PRO:HD2	2.22	0.40
1:B:34:LEU:O	1:B:38:GLN:HG3	2.21	0.40
1:D:6:PRO:HG2	1:D:37:LEU:HD13	2.02	0.40
1:C:640:GLU:O	1:C:643:PRO:HD2	2.22	0.40
1:C:865:ARG:N	1:C:866:PRO:HD2	2.37	0.40
1:A:438:GLU:OE2	1:A:480:THR:HG21	2.22	0.40
1:B:865:ARG:N	1:B:866:PRO:HD2	2.36	0.40
1:D:136:ASP:HB3	1:D:139:SER:OG	2.21	0.40
1:C:804:HIS:CD2	1:C:808:ALA:HB2	2.57	0.40
1:B:303:CYS:HB3	1:B:345:PHE:CE1	2.56	0.40
1:D:581:LEU:HG	1:D:637:VAL:HG11	2.02	0.40
1:B:127:GLN:O	1:B:131:GLU:HG2	2.21	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%)	46 80
1	B	793/820 (97%)	766 (97%)	27 (3%)	44 79
1	C	793/820 (97%)	767 (97%)	26 (3%)	45 80
1	D	794/820 (97%)	769 (97%)	25 (3%)	47 81
All	All	3173/3280 (97%)	3070 (97%)	103 (3%)	46 80

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 carbohydrates 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	A	1923	-	7,7,7	0.58	0	4,8,8	1.05	1 (25%)
2	DTT	B	1923	-	7,7,7	0.57	0	4,8,8	0.69	0
2	DTT	C	1923	-	7,7,7	0.58	0	4,8,8	0.76	0
2	DTT	D	1923	-	7,7,7	0.59	0	4,8,8	0.29	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	-	-	0/8/8/8	0/0/0/0
2	DTT	B	1923	-	-	0/8/8/8	0/0/0/0
2	DTT	C	1923	-	-	0/8/8/8	0/0/0/0
2	DTT	D	1923	-	-	0/8/8/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1923	DTT	C2-C1-S1	-2.06	110.49	113.91

There are no chirality outliers.

There are no torsion outliers.

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	B	1923	DTT	1	0
2	C	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, 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%)	0.35	45 (5%)	32	18	53, 88, 126, 162	0
1	B	889/923 (96%)	0.33	30 (3%)	49	30	54, 88, 125, 163	0
1	C	889/923 (96%)	0.38	37 (4%)	40	23	54, 88, 124, 163	0
1	D	890/923 (96%)	0.31	32 (3%)	46	28	53, 88, 125, 162	0
All	All	3557/3692 (96%)	0.34	144 (4%)	42	25	53, 88, 125, 163	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	57	VAL	5.0
1	A	452	ASP	4.6
1	B	594	LYS	4.5
1	C	22	PRO	4.4
1	D	548	LEU	4.1
1	B	468	ARG	4.1
1	A	221	ASN	3.9
1	B	626	VAL	3.9
1	B	42	HIS	3.8
1	C	171	GLU	3.8
1	A	795	VAL	3.7
1	A	849	THR	3.7
1	D	455	ASN	3.6
1	B	455	ASN	3.6
1	A	636	LYS	3.6
1	B	714	GLU	3.6
1	B	161	ILE	3.6
1	A	171	GLU	3.5
1	B	849	THR	3.3
1	D	626	VAL	3.2
1	A	196	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	161	ILE	3.2
1	B	575	ASP	3.2
1	C	147	LEU	3.1
1	D	385	ASP	3.1
1	A	260	GLU	3.1
1	D	492	VAL	3.1
1	C	499	LEU	3.1
1	B	59	SER	3.1
1	C	158	SER	3.0
1	A	79	PRO	3.0
1	C	316	GLN	3.0
1	C	175	PHE	3.0
1	D	59	SER	3.0
1	D	577	ILE	2.9
1	C	257	GLU	2.9
1	C	157	ARG	2.9
1	A	625	ILE	2.9
1	D	636	LYS	2.9
1	D	590	MET	2.9
1	B	579	GLU	2.9
1	B	890	VAL	2.9
1	C	189	GLU	2.8
1	A	845	LEU	2.8
1	D	21	ASP	2.8
1	D	382	LEU	2.7
1	A	574	LEU	2.7
1	A	848	TYR	2.7
1	B	57	VAL	2.7
1	C	79	PRO	2.7
1	C	642	TRP	2.7
1	A	920	ARG	2.7
1	A	161	ILE	2.7
1	C	534	MET	2.7
1	B	552	LEU	2.6
1	B	185	MET	2.6
1	D	468	ARG	2.6
1	A	469	LEU	2.6
1	A	577	ILE	2.6
1	A	8	LEU	2.6
1	D	595	LEU	2.6
1	B	267	MET	2.6
1	C	55	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	180	VAL	2.6
1	C	170	ILE	2.5
1	D	16	GLN	2.5
1	C	920	ARG	2.5
1	B	815	PHE	2.5
1	C	125	CYS	2.5
1	A	420	PHE	2.5
1	A	125	CYS	2.5
1	A	429	GLU	2.4
1	B	9	GLN	2.4
1	A	57	VAL	2.4
1	A	60	CYS	2.4
1	A	611	PHE	2.4
1	B	60	CYS	2.4
1	A	299	PHE	2.4
1	C	124	GLY	2.4
1	C	571	ARG	2.4
1	D	315	GLY	2.3
1	A	492	VAL	2.3
1	B	625	ILE	2.3
1	D	161	ILE	2.3
1	A	20	HIS	2.3
1	D	20	HIS	2.3
1	A	48	ASP	2.3
1	C	919	THR	2.3
1	B	572	LEU	2.3
1	A	117	LEU	2.3
1	C	636	LYS	2.3
1	C	789	ARG	2.2
1	A	123	LYS	2.2
1	A	175	PHE	2.2
1	A	316	GLN	2.2
1	C	318	LEU	2.2
1	D	316	GLN	2.2
1	D	609	THR	2.2
1	B	580	CYS	2.2
1	C	594	LYS	2.2
1	C	213	VAL	2.2
1	A	572	LEU	2.2
1	B	316	GLN	2.2
1	C	143	LEU	2.2
1	C	922	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	104	ILE	2.2
1	A	144	LEU	2.2
1	B	452	ASP	2.2
1	C	734	GLN	2.2
1	D	157	ARG	2.2
1	B	238	SER	2.1
1	D	538	PHE	2.1
1	C	577	ILE	2.1
1	A	491	VAL	2.1
1	C	57	VAL	2.1
1	C	649	LEU	2.1
1	D	890	VAL	2.1
1	A	552	LEU	2.1
1	C	587	VAL	2.1
1	D	78	LEU	2.1
1	B	16	GLN	2.1
1	A	135	ASN	2.1
1	B	257	GLU	2.1
1	C	469	LEU	2.1
1	D	155	HIS	2.1
1	C	21	ASP	2.1
1	B	404	SER	2.1
1	D	920	ARG	2.1
1	D	456	ASN	2.1
1	A	146	ILE	2.0
1	C	743	GLN	2.0
1	A	27	LYS	2.0
1	D	714	GLU	2.0
1	D	176	TYR	2.0
1	A	576	LYS	2.0
1	D	579	GLU	2.0
1	C	788	HIS	2.0
1	A	154	VAL	2.0
1	A	919	THR	2.0
1	D	318	LEU	2.0
1	B	454	GLU	2.0
1	D	196	LYS	2.0
1	A	548	LEU	2.0
1	A	82	SER	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	DTT	C	1923	8/8	0.77	0.32	4.48	85,111,121,143	0
2	DTT	A	1923	8/8	0.84	0.28	1.56	72,99,109,126	0
2	DTT	B	1923	8/8	0.89	0.23	1.55	92,104,134,144	0
2	DTT	D	1923	8/8	0.87	0.23	0.80	79,94,108,114	0

6.5 Other polymers (i)

There are no such residues in this entry.