Full wwPDB X-ray Structure Validation Report ⓘ

Aug 12, 2024 – 08:59 PM EDT

PDB ID	:	8TTA
Title	:	Structure of retromer VPS29-VPS35 (483-796) complexed with Fam21A repeat 21 (1328-1341)
Authors	:	Chen, K.-E.; Guo, Q.; Collins, B.M.
Deposited on	:	2023-08-13
Resolution	:	3.46 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:

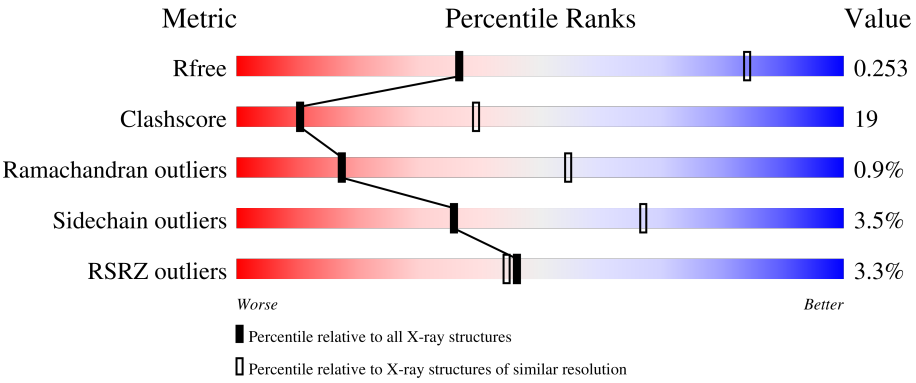
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 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.



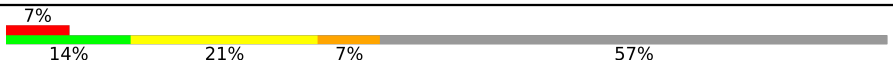
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 <=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	192	2% 56% 36% • 5%
1	C	192	7% 54% 42% • •
2	B	314	% 61% 34% • •
2	D	314	2% 57% 36% • 5%
3	E	14	21% 36% 14% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	14	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7948 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 Vacuolar protein sorting-associated protein 29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1456	940	246	264	6			
1	C	188	Total	C	N	O	S	0	0	0
			1497	965	254	272	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q9QZ88
A	-8	SER	-	expression tag	UNP Q9QZ88
A	-7	PRO	-	expression tag	UNP Q9QZ88
A	-6	GLU	-	expression tag	UNP Q9QZ88
A	-5	PHE	-	expression tag	UNP Q9QZ88
A	-4	GLY	-	expression tag	UNP Q9QZ88
A	-3	THR	-	expression tag	UNP Q9QZ88
A	-2	ARG	-	expression tag	UNP Q9QZ88
A	-1	ASP	-	expression tag	UNP Q9QZ88
A	0	ARG	-	expression tag	UNP Q9QZ88
C	-9	GLY	-	expression tag	UNP Q9QZ88
C	-8	SER	-	expression tag	UNP Q9QZ88
C	-7	PRO	-	expression tag	UNP Q9QZ88
C	-6	GLU	-	expression tag	UNP Q9QZ88
C	-5	PHE	-	expression tag	UNP Q9QZ88
C	-4	GLY	-	expression tag	UNP Q9QZ88
C	-3	THR	-	expression tag	UNP Q9QZ88
C	-2	ARG	-	expression tag	UNP Q9QZ88
C	-1	ASP	-	expression tag	UNP Q9QZ88
C	0	ARG	-	expression tag	UNP Q9QZ88

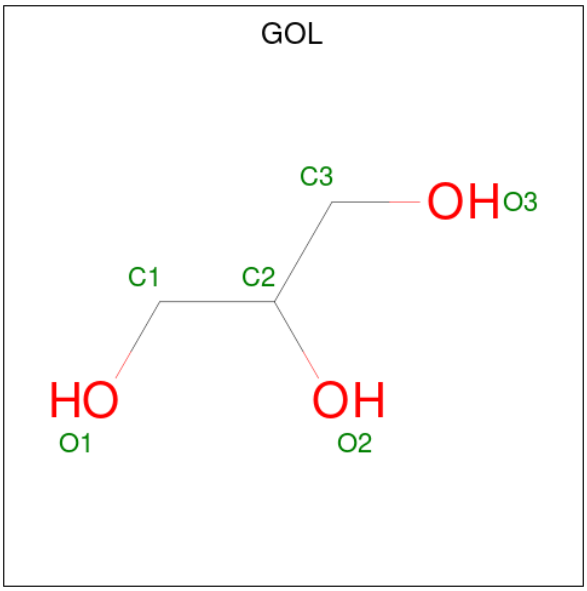
- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	301	Total	C	N	O	S	0	0	0
			2438	1544	428	455	11			
2	D	299	Total	C	N	O	S	7	0	0
			2418	1530	425	452	11			

- Molecule 3 is a protein called SER-ASN-ILE-PHE-ASP-ASP-PRO-LEU-ASN-ALA-PHE-GLY-GLY-GLN.

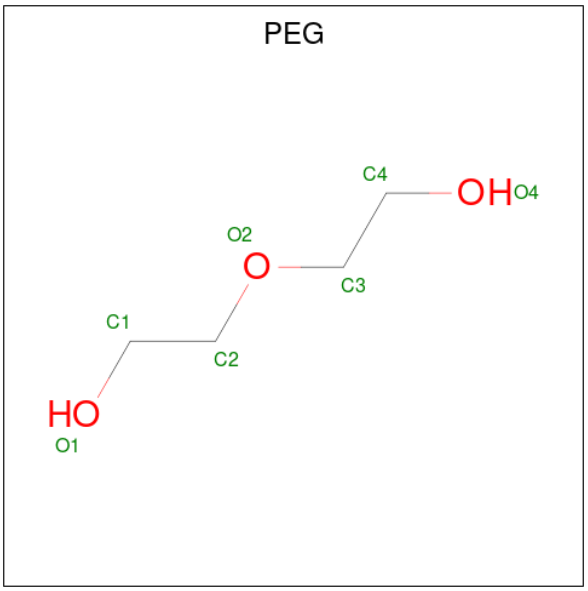
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	7	Total	C	N	O	0	0	0
			55	35	8	12			
3	F	6	Total	C	N	O	0	0	0
			44	26	7	11			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



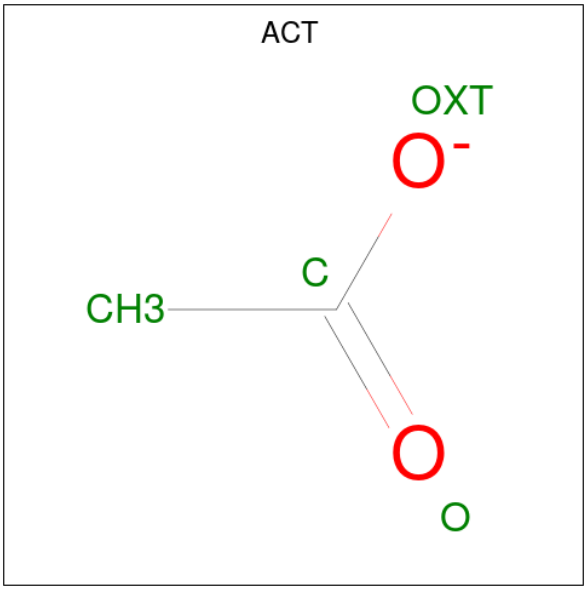
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

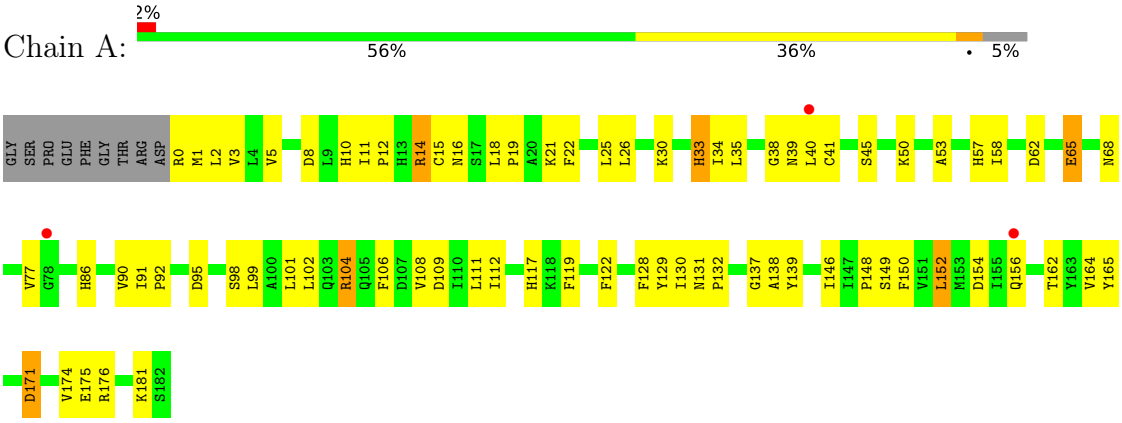
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total O 3 3	0	0
7	B	1	Total O 1 1	0	0
7	C	1	Total O 1 1	0	0
7	D	5	Total O 5 5	0	0

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.

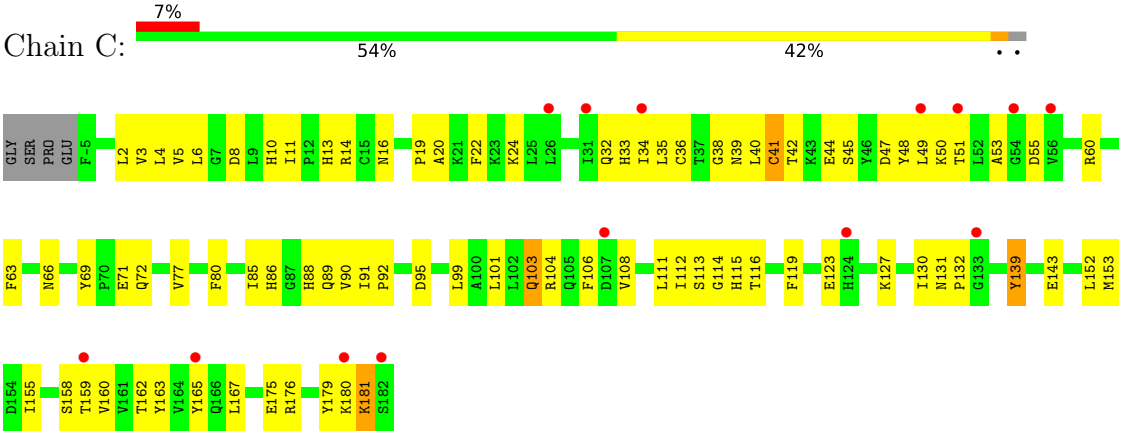
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



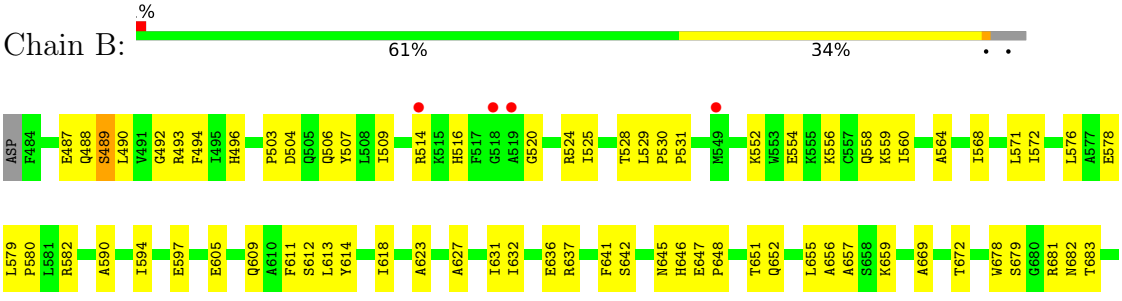
• Molecule 1: Vacuolar protein sorting-associated protein 29

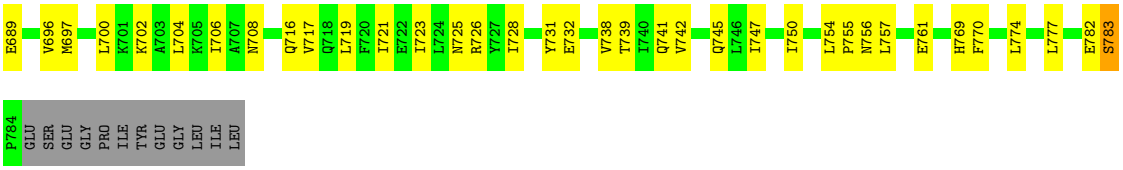
Chain C:



• Molecule 2: Vacuolar protein sorting-associated protein 35

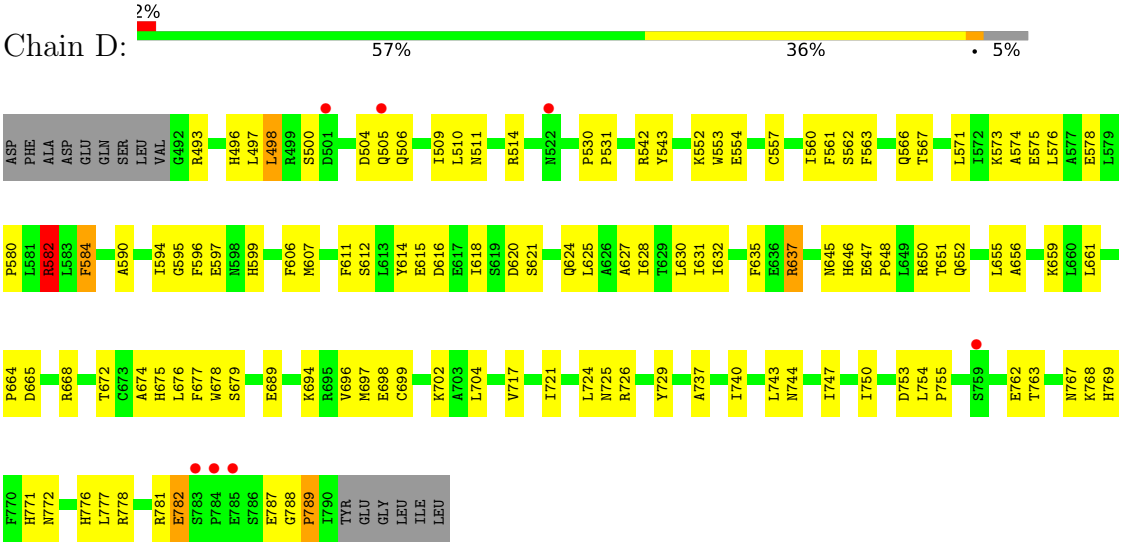
Chain B:





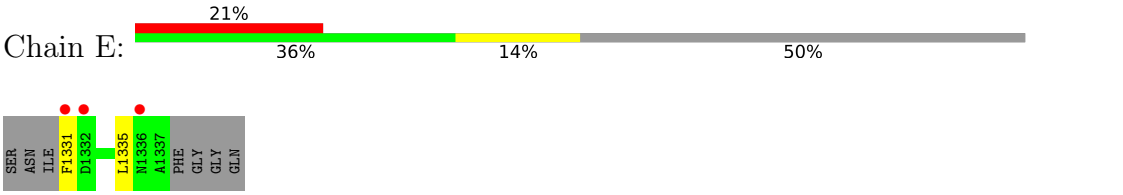
• Molecule 2: Vacuolar protein sorting-associated protein 35

Chain D:



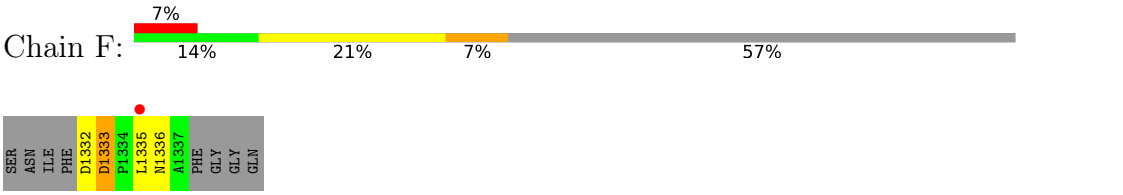
• Molecule 3: SER-ASN-ILE-PHE-ASP-ASP-PRO-LEU-ASN-ALA-PHE-GLY-GLY-GLN

Chain E:



• Molecule 3: SER-ASN-ILE-PHE-ASP-ASP-PRO-LEU-ASN-ALA-PHE-GLY-GLY-GLN

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.73Å 165.58Å 68.00Å 90.00° 117.51° 90.00°	Depositor
Resolution (Å)	48.75 – 3.46 48.75 – 3.46	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.75-3.46) 99.1 (48.75-3.46)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.221 , 0.253 0.223 , 0.253	Depositor DCC
R_{free} test set	787 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	77.6	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 73.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7948	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: GOL, PEG, ACT

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	0/1489	0.62	0/2018
1	C	0.30	0/1531	0.64	0/2074
2	B	0.30	0/2486	0.63	0/3347
2	D	0.34	0/2466	0.64	0/3320
3	E	0.38	0/56	0.62	0/76
3	F	0.32	0/44	0.78	0/60
All	All	0.32	0/8072	0.64	0/10895

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
2	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ARG	Sidechain
1	A	14	ARG	Sidechain
1	C	104	ARG	Sidechain
2	D	582	ARG	Sidechain

5.2 Too-close contacts (i)

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	1456	0	1470	69	0
1	C	1497	0	1506	69	0
2	B	2438	0	2415	78	0
2	D	2418	0	2396	90	0
3	E	55	0	45	3	0
3	F	44	0	36	2	0
4	B	12	0	16	0	0
5	C	7	0	10	1	0
5	D	7	0	10	3	0
6	D	4	0	3	0	0
7	A	3	0	0	1	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	5	0	0	0	0
All	All	7948	0	7907	294	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 19.

All (294) 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)
2:D:724:LEU:HD11	2:D:747:ILE:HG22	1.45	0.95
1:A:117:HIS:HB3	1:A:146:ILE:HD11	1.50	0.94
1:A:3:VAL:HG12	1:A:33:HIS:HB2	1.55	0.88
1:A:10:HIS:HE1	1:A:14:ARG:HH21	1.19	0.87
1:C:22:PHE:HE1	1:C:167:LEU:HB2	1.41	0.85
1:C:80:PHE:HE1	1:C:181:LYS:HG3	1.39	0.85
1:A:106:PHE:HB3	1:A:108:VAL:HG13	1.62	0.82
2:B:646:HIS:HD2	2:B:682:ASN:HB3	1.46	0.80
1:A:112:ILE:HG22	1:A:130:ILE:HB	1.63	0.79
1:C:8:ASP:H	1:C:38:GLY:HA3	1.49	0.78
1:C:40:LEU:HD12	1:C:42:THR:H	1.49	0.78
1:A:10:HIS:CE1	1:A:14:ARG:HH21	2.02	0.77
1:A:10:HIS:CE1	1:A:14:ARG:NH2	2.54	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:747:ILE:CD1	2:B:774:LEU:HD21	2.17	0.75
2:D:717:VAL:O	2:D:721:ILE:HD12	1.87	0.75
2:D:621:SER:HB2	2:D:661:LEU:HD12	1.68	0.74
1:A:10:HIS:HE1	1:A:14:ARG:NH2	1.86	0.73
1:A:14:ARG:HD3	1:A:139:TYR:HB3	1.71	0.73
2:D:514:ARG:HD2	2:D:563:PHE:HE1	1.52	0.73
2:B:605:GLU:OE2	2:B:609:GLN:NE2	2.22	0.72
1:A:101:LEU:HD13	1:A:104:ARG:HH12	1.56	0.71
2:D:650:ARG:HD3	2:D:677:PHE:CE1	2.25	0.71
2:B:556:LYS:O	2:B:560:ILE:HG12	1.89	0.71
2:D:496:HIS:CE1	2:D:498:LEU:HD22	2.24	0.71
2:B:741:GLN:O	2:B:745:GLN:HG3	1.90	0.70
1:A:137:GLY:HA3	1:A:148:PRO:HG3	1.74	0.69
1:C:80:PHE:HD1	1:C:181:LYS:HZ3	1.41	0.69
2:B:642:SER:O	2:B:646:HIS:N	2.25	0.68
1:C:80:PHE:CE1	1:C:181:LYS:HG3	2.26	0.67
1:A:62:ASP:O	2:B:582:ARG:NH1	2.27	0.67
2:B:700:LEU:HD21	2:B:726:ARG:HB3	1.77	0.66
1:C:60:ARG:HG3	1:C:69:TYR:O	1.93	0.66
1:A:68:ASN:OD1	2:D:553:TRP:NE1	2.28	0.66
1:C:153:MET:HB3	1:C:162:THR:HG22	1.77	0.66
2:D:655:LEU:HD21	2:D:659:LYS:HD2	1.78	0.66
1:A:128:PHE:CE2	1:A:130:ILE:HD11	2.31	0.65
1:A:176:ARG:HB3	3:E:1331:PHE:HZ	1.60	0.65
1:A:138:ALA:O	1:A:146:ILE:HD13	1.97	0.65
1:C:14:ARG:NH1	1:C:139:TYR:O	2.29	0.65
1:C:92:PRO:HB2	1:C:95:ASP:HB2	1.78	0.65
1:A:101:LEU:HD13	2:B:725:ASN:HB3	1.79	0.65
2:B:646:HIS:CD2	2:B:682:ASN:HB3	2.30	0.65
2:B:627:ALA:O	2:B:631:ILE:HG13	1.98	0.64
2:D:674:ALA:HB1	2:D:696:VAL:HG13	1.79	0.64
1:C:116:THR:OG1	1:C:131:ASN:ND2	2.30	0.64
2:B:782:GLU:HG2	2:B:783:SER:N	2.12	0.64
2:B:754:LEU:HB3	2:B:755:PRO:HD3	1.79	0.63
1:A:8:ASP:H	1:A:38:GLY:HA3	1.63	0.63
2:D:500:SER:O	2:D:542:ARG:NH2	2.31	0.63
2:B:564:ALA:O	2:B:568:ILE:HG13	1.98	0.63
1:A:104:ARG:NH1	2:B:725:ASN:OD1	2.32	0.63
1:C:22:PHE:CE1	1:C:167:LEU:HB2	2.31	0.63
1:C:106:PHE:HB3	1:C:108:VAL:HG13	1.81	0.63
1:C:13:HIS:HE1	1:C:41:CYS:HB2	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:781:ARG:O	2:D:782:GLU:HB2	1.98	0.62
2:D:542:ARG:HH11	2:D:542:ARG:HB3	1.64	0.62
2:D:557:CYS:HA	2:D:560:ILE:HG22	1.81	0.62
1:C:88:HIS:HB3	1:C:115:HIS:ND1	2.15	0.62
1:C:34:ILE:HG21	1:C:49:LEU:HD12	1.82	0.61
2:B:655:LEU:HB3	2:B:659:LYS:HE3	1.83	0.61
2:D:576:LEU:HG	2:D:580:PRO:HD3	1.82	0.61
1:C:60:ARG:HB2	1:C:71:GLU:HA	1.81	0.61
2:D:627:ALA:O	2:D:631:ILE:HG13	2.00	0.61
1:A:22:PHE:O	1:A:26:LEU:HD12	2.01	0.61
1:A:21:LYS:NZ	1:A:171:ASP:OD1	2.34	0.60
2:D:530:PRO:HB2	2:D:531:PRO:HD3	1.83	0.60
2:D:590:ALA:O	2:D:594:ILE:HG13	2.00	0.60
1:A:2:LEU:HD21	1:A:30:LYS:O	2.01	0.60
2:B:572:ILE:HD11	2:B:613:LEU:HD11	1.83	0.60
2:B:618:ILE:HD11	2:B:623:ALA:HB1	1.83	0.60
1:C:47:ASP:O	1:C:51:THR:HG23	2.02	0.60
2:D:628:ILE:O	2:D:632:ILE:HG13	2.02	0.60
2:B:747:ILE:HG13	2:B:770:PHE:HZ	1.66	0.60
2:D:584:PHE:HD1	2:D:606:PHE:HD1	1.50	0.59
1:C:119:PHE:HA	1:C:131:ASN:O	2.01	0.59
2:D:655:LEU:HD23	2:D:655:LEU:C	2.23	0.59
2:B:530:PRO:HB2	2:B:531:PRO:HD3	1.85	0.59
2:D:542:ARG:HB3	2:D:542:ARG:NH1	2.18	0.59
2:B:507:TYR:CE2	2:B:559:LYS:HD3	2.38	0.59
1:C:88:HIS:HD2	2:D:630:LEU:HD21	1.66	0.59
2:D:743:LEU:O	2:D:747:ILE:HG23	2.03	0.58
1:A:176:ARG:CB	3:E:1331:PHE:HZ	2.15	0.58
2:B:697:MET:SD	2:B:738:VAL:HG22	2.44	0.58
1:C:44:GLU:OE1	2:D:493:ARG:NH1	2.36	0.58
2:D:724:LEU:HD12	2:D:750:ILE:HD12	1.85	0.58
1:A:101:LEU:CD1	2:B:725:ASN:HB3	2.34	0.57
2:B:651:THR:O	2:B:655:LEU:HG	2.04	0.57
2:D:582:ARG:H	2:D:582:ARG:HD2	1.69	0.57
2:D:754:LEU:HB3	2:D:755:PRO:HD3	1.86	0.57
2:B:717:VAL:O	2:B:721:ILE:HG13	2.04	0.57
2:B:747:ILE:HD11	2:B:774:LEU:HD21	1.86	0.57
1:C:20:ALA:O	1:C:24:LYS:HG2	2.05	0.57
1:C:101:LEU:HD13	2:D:725:ASN:HB3	1.86	0.57
2:D:496:HIS:CG	2:D:498:LEU:HB3	2.40	0.57
2:D:615:GLU:OE2	2:D:652:GLN:NE2	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LEU:HB2	1:C:45:SER:HB2	1.86	0.56
2:D:614:TYR:CE2	2:D:656:ALA:HB1	2.41	0.56
2:B:632:ILE:HG21	2:B:672:THR:HG22	1.89	0.55
2:B:708:ASN:HA	2:B:716:GLN:NE2	2.21	0.55
2:D:562:SER:O	2:D:566:GLN:HG3	2.06	0.55
2:D:574:ALA:O	2:D:576:LEU:N	2.40	0.55
2:D:596:PHE:O	2:D:599:HIS:ND1	2.34	0.55
1:A:38:GLY:HA2	1:A:86:HIS:CD2	2.42	0.55
1:A:119:PHE:HA	1:A:131:ASN:O	2.06	0.55
2:B:552:LYS:O	2:B:556:LYS:HG3	2.06	0.55
1:A:50:LYS:NZ	2:D:597:GLU:OE2	2.38	0.55
1:C:66:ASN:HB3	1:C:69:TYR:CE2	2.42	0.55
2:D:698:GLU:O	2:D:702:LYS:HB2	2.07	0.54
2:B:747:ILE:HG13	2:B:770:PHE:CZ	2.43	0.54
1:C:92:PRO:HB3	2:D:637:ARG:HH21	1.72	0.54
1:A:101:LEU:CD1	1:A:104:ARG:HH12	2.20	0.54
2:B:750:ILE:O	2:B:754:LEU:HB2	2.08	0.54
2:D:675:HIS:HE1	2:D:729:TYR:HE2	1.55	0.54
1:A:0:ARG:NH2	1:A:154:ASP:OD2	2.38	0.54
2:B:609:GLN:O	2:B:613:LEU:HD12	2.07	0.54
2:D:787:GLU:HB3	2:D:789:PRO:HD3	1.89	0.54
2:B:719:LEU:O	2:B:723:ILE:HG13	2.08	0.53
1:C:80:PHE:HD1	1:C:181:LYS:NZ	2.06	0.53
1:C:8:ASP:N	1:C:38:GLY:HA3	2.20	0.53
1:C:77:VAL:HG11	1:C:155:ILE:HD12	1.91	0.53
1:A:40:LEU:HD21	1:A:58:ILE:HD13	1.90	0.53
2:B:578:GLU:HG2	2:B:618:ILE:HD12	1.90	0.52
2:B:657:ALA:HB1	2:B:669:ALA:HB1	1.90	0.52
2:B:489:SER:O	2:B:493:ARG:N	2.41	0.52
2:B:503:PRO:HA	2:B:506:GLN:HB2	1.91	0.52
2:D:678:TRP:HB2	2:D:696:VAL:HG21	1.90	0.52
1:C:5:VAL:HG12	1:C:132:PRO:HG3	1.92	0.52
1:A:5:VAL:HG21	1:A:112:ILE:HD12	1.92	0.52
1:A:16:ASN:OD1	2:B:496:HIS:HB2	2.09	0.52
1:C:6:LEU:HD21	1:C:49:LEU:HD11	1.90	0.52
2:D:647:GLU:O	2:D:651:THR:HG23	2.09	0.52
2:D:768:LYS:HD2	2:D:772:ASN:OD1	2.10	0.52
2:D:788:GLY:N	2:D:789:PRO:HD3	2.25	0.51
1:C:90:VAL:HG11	1:C:99:LEU:HD23	1.91	0.51
2:B:721:ILE:HD13	2:B:770:PHE:HB2	1.93	0.51
2:B:704:LEU:HG	2:B:723:ILE:HG21	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:514:ARG:HH21	2:D:567:THR:HA	1.75	0.51
2:B:702:LYS:O	2:B:706:ILE:HG13	2.11	0.51
2:B:750:ILE:HG21	2:B:770:PHE:CD2	2.45	0.51
1:A:122:PHE:HE1	1:A:129:TYR:HD2	1.59	0.51
2:B:678:TRP:HB2	2:B:696:VAL:HG21	1.92	0.51
2:B:739:THR:OG1	2:B:742:VAL:HG23	2.11	0.51
1:C:5:VAL:HG22	1:C:35:LEU:HB2	1.92	0.51
2:B:636:GLU:OE2	2:B:679:SER:OG	2.27	0.50
1:C:39:ASN:HD21	1:C:86:HIS:CE1	2.30	0.50
1:C:3:VAL:O	1:C:152:LEU:HB2	2.12	0.50
2:B:525:ILE:HA	2:B:528:THR:HB	1.93	0.50
1:A:39:ASN:ND2	1:A:62:ASP:OD1	2.45	0.50
2:B:516:HIS:C	2:B:516:HIS:CD2	2.84	0.50
2:B:614:TYR:O	2:B:618:ILE:HG22	2.12	0.49
1:C:5:VAL:HG11	1:C:112:ILE:HD12	1.94	0.49
1:C:101:LEU:CD1	2:D:725:ASN:HB3	2.41	0.49
2:B:590:ALA:O	2:B:594:ILE:HG13	2.12	0.49
2:B:696:VAL:O	2:B:700:LEU:HD12	2.12	0.49
2:B:636:GLU:OE1	2:B:637:ARG:NE	2.44	0.49
1:C:85:ILE:HD11	1:C:89:GLN:HE21	1.76	0.49
2:D:554:GLU:OE1	2:D:597:GLU:N	2.42	0.49
1:A:132:PRO:O	1:A:149:SER:OG	2.30	0.49
3:F:1332:ASP:O	3:F:1333:ASP:HB3	2.12	0.49
2:B:708:ASN:HA	2:B:716:GLN:HE21	1.78	0.49
1:C:160:VAL:HG12	1:C:179:TYR:O	2.11	0.49
1:A:5:VAL:HA	1:A:35:LEU:O	2.11	0.49
2:B:572:ILE:HG12	2:B:613:LEU:HD21	1.94	0.49
1:C:8:ASP:H	1:C:38:GLY:CA	2.23	0.49
1:C:159:THR:OG1	1:C:180:LYS:HE2	2.12	0.49
2:B:728:ILE:HD13	2:B:777:LEU:HD21	1.95	0.49
2:D:614:TYR:HE2	2:D:656:ALA:HB1	1.77	0.48
2:D:578:GLU:HG2	2:D:618:ILE:HD12	1.94	0.48
1:A:2:LEU:HD23	1:A:2:LEU:H	1.78	0.48
2:D:675:HIS:CE1	2:D:729:TYR:HE2	2.31	0.48
2:D:679:SER:O	2:D:689:GLU:HG2	2.13	0.48
1:A:16:ASN:HB3	2:B:492:GLY:O	2.12	0.48
1:A:19:PRO:HD2	1:A:22:PHE:HB2	1.95	0.48
1:C:91:ILE:HD12	2:D:672:THR:HG23	1.95	0.48
2:B:507:TYR:HE2	2:B:559:LYS:HD3	1.78	0.48
1:C:19:PRO:HD2	1:C:22:PHE:HB2	1.95	0.47
2:D:650:ARG:HD3	2:D:677:PHE:HE1	1.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG11	1:A:99:LEU:HG	1.97	0.47
1:A:109:ASP:OD2	1:A:181:LYS:NZ	2.41	0.47
1:A:128:PHE:HE2	1:A:162:THR:HG21	1.78	0.47
1:A:21:LYS:HZ2	1:A:171:ASP:HA	1.80	0.47
1:C:3:VAL:HG22	1:C:33:HIS:HB2	1.96	0.47
1:C:41:CYS:HB3	1:C:63:PHE:O	2.15	0.47
1:C:112:ILE:HD13	1:C:130:ILE:HB	1.97	0.47
2:D:655:LEU:HD23	2:D:655:LEU:O	2.15	0.47
2:B:641:PHE:O	2:B:683:THR:HG23	2.15	0.47
1:C:152:LEU:CD2	1:C:165:TYR:HE1	2.27	0.47
1:C:152:LEU:HD22	1:C:165:TYR:HE1	1.79	0.46
3:F:1335:LEU:HB3	3:F:1336:ASN:H	1.61	0.46
1:A:40:LEU:HB2	1:A:45:SER:HB2	1.98	0.46
1:C:114:GLY:HA2	1:C:131:ASN:OD1	2.15	0.46
1:C:163:TYR:OH	1:C:176:ARG:NH2	2.31	0.46
1:A:11:ILE:HA	1:A:15:CYS:O	2.15	0.46
1:C:47:ASP:HA	1:C:50:LYS:HB2	1.97	0.46
1:C:163:TYR:HA	1:C:175:GLU:O	2.16	0.46
2:D:697:MET:SD	2:D:737:ALA:O	2.74	0.46
2:D:509:ILE:HG13	2:D:510:LEU:N	2.31	0.46
1:A:2:LEU:HA	1:A:154:ASP:HA	1.97	0.46
2:D:571:LEU:HD23	2:D:571:LEU:HA	1.76	0.46
2:B:645:ASN:O	2:B:648:PRO:HD2	2.16	0.46
1:C:34:ILE:HG12	1:C:53:ALA:HB3	1.98	0.46
2:B:554:GLU:HG2	2:B:597:GLU:H	1.81	0.45
2:D:625:LEU:HD12	2:D:665:ASP:OD1	2.16	0.45
1:A:35:LEU:HD22	1:A:57:HIS:HB2	1.99	0.45
1:C:130:ILE:HD11	1:C:162:THR:HG21	1.98	0.45
2:D:612:SER:O	2:D:616:ASP:HB2	2.16	0.45
1:A:102:LEU:HD23	1:A:111:LEU:HD11	1.98	0.45
2:B:487:GLU:O	2:B:490:LEU:HB3	2.17	0.45
1:A:22:PHE:CE2	1:A:150:PHE:HD1	2.35	0.45
2:B:525:ILE:HB	2:B:529:LEU:HG	1.97	0.45
2:B:728:ILE:O	2:B:732:GLU:HG3	2.15	0.45
1:A:21:LYS:O	1:A:25:LEU:HG	2.16	0.45
1:C:10:HIS:N	1:C:39:ASN:O	2.39	0.45
1:C:11:ILE:HG22	1:C:42:THR:HG21	1.98	0.45
1:C:103:GLN:HB2	1:C:111:LEU:HD12	1.99	0.44
2:D:496:HIS:ND1	2:D:498:LEU:HB3	2.32	0.44
2:D:655:LEU:C	2:D:655:LEU:CD2	2.85	0.44
2:D:777:LEU:HD23	2:D:777:LEU:HA	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD12	1:A:18:LEU:H	1.83	0.44
2:D:778:ARG:HG2	2:D:781:ARG:HH22	1.82	0.44
2:B:747:ILE:HD12	2:B:774:LEU:HD21	1.98	0.44
2:D:514:ARG:HD2	2:D:563:PHE:CE1	2.42	0.44
1:A:14:ARG:NH1	1:A:139:TYR:O	2.51	0.44
1:C:6:LEU:O	1:C:36:CYS:HA	2.17	0.44
2:D:504:ASP:HA	2:D:543:TYR:OH	2.17	0.44
2:D:506:GLN:HA	2:D:509:ILE:HG12	1.99	0.44
2:D:620:ASP:O	2:D:624:GLN:N	2.45	0.44
1:A:34:ILE:HG13	1:A:53:ALA:HB3	1.99	0.44
2:B:756:ASN:O	2:B:757:LEU:HD23	2.17	0.44
2:D:704:LEU:HD23	2:D:704:LEU:HA	1.83	0.44
1:A:92:PRO:HB2	1:A:95:ASP:HB2	1.98	0.44
1:C:42:THR:HG23	1:C:45:SER:H	1.82	0.44
1:A:3:VAL:O	1:A:152:LEU:HB2	2.18	0.43
1:A:25:LEU:O	3:E:1335:LEU:HD13	2.18	0.43
2:D:763:THR:O	2:D:767:ASN:ND2	2.46	0.43
1:A:129:TYR:O	1:A:130:ILE:HD13	2.18	0.43
1:C:115:HIS:CD2	1:C:115:HIS:O	2.71	0.43
1:A:41:CYS:O	1:A:65:GLU:HG3	2.18	0.43
2:B:520:GLY:O	2:B:524:ARG:NE	2.45	0.43
2:D:607:MET:HB2	2:D:607:MET:HE2	1.62	0.43
1:A:175:GLU:HG2	1:A:176:ARG:N	2.34	0.43
2:D:776:HIS:C	2:D:776:HIS:CD2	2.90	0.43
2:B:571:LEU:O	2:B:576:LEU:HB2	2.18	0.43
2:D:645:ASN:O	2:D:648:PRO:HD2	2.18	0.43
2:D:717:VAL:HG22	2:D:753:ASP:OD2	2.19	0.43
2:B:494:PHE:HZ	2:B:509:ILE:HG22	1.84	0.43
2:D:584:PHE:HD1	2:D:606:PHE:CD1	2.35	0.43
2:B:645:ASN:C	2:B:648:PRO:HD2	2.39	0.43
2:D:582:ARG:HD2	2:D:582:ARG:N	2.33	0.43
2:D:675:HIS:HE1	2:D:729:TYR:CE2	2.35	0.42
1:C:2:LEU:HD23	1:C:32:GLN:OE1	2.19	0.42
2:B:647:GLU:O	2:B:651:THR:HG23	2.20	0.42
2:D:620:ASP:O	2:D:624:GLN:HB2	2.18	0.42
2:D:744:ASN:OD1	2:D:789:PRO:HB2	2.19	0.42
1:A:19:PRO:O	1:A:22:PHE:HB2	2.19	0.42
1:A:122:PHE:CE1	1:A:129:TYR:HD2	2.36	0.42
1:A:1:MET:SD	1:A:77:VAL:HG12	2.60	0.42
1:A:164:VAL:O	1:A:174:VAL:HA	2.20	0.42
2:B:614:TYR:CE2	2:B:656:ALA:HB1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ILE:H	1:C:155:ILE:HG13	1.64	0.41
2:D:767:ASN:O	2:D:771:HIS:ND1	2.53	0.41
2:B:554:GLU:O	2:B:558:GLN:HG3	2.20	0.41
2:D:611:PHE:O	2:D:615:GLU:HG3	2.20	0.41
1:C:72:GLN:OE1	5:C:201:PEG:H22	2.20	0.41
1:A:40:LEU:HD12	1:A:45:SER:C	2.41	0.41
1:C:4:LEU:HD23	1:C:34:ILE:HD12	2.03	0.41
2:D:595:GLY:HA2	2:D:599:HIS:CE1	2.55	0.41
2:D:496:HIS:O	2:D:497:LEU:HB2	2.19	0.41
2:D:699:CYS:SG	5:D:802:PEG:H32	2.61	0.41
1:A:12:PRO:HA	1:A:15:CYS:O	2.20	0.41
2:B:579:LEU:HB3	2:B:580:PRO:HD3	2.02	0.41
1:A:152:LEU:HD23	1:A:165:TYR:HE1	1.85	0.41
1:C:90:VAL:HG11	1:C:99:LEU:CD2	2.51	0.41
2:D:571:LEU:HB3	2:D:576:LEU:HD23	2.03	0.41
1:A:91:ILE:HD12	2:B:672:THR:CG2	2.51	0.41
2:B:611:PHE:CD1	2:B:652:GLN:HG2	2.56	0.41
1:C:143:GLU:HA	1:C:143:GLU:OE1	2.20	0.41
2:D:664:PRO:O	2:D:668:ARG:HG3	2.21	0.41
1:A:68:ASN:ND2	7:A:201:HOH:O	2.53	0.41
2:B:576:LEU:HD23	2:B:576:LEU:HA	1.90	0.41
1:C:80:PHE:CD2	1:C:155:ILE:HG23	2.56	0.41
1:C:85:ILE:O	1:C:113:SER:HA	2.21	0.41
2:D:694:LYS:HG3	2:D:694:LYS:O	2.21	0.41
1:A:14:ARG:NH1	1:A:139:TYR:CD2	2.88	0.40
2:B:777:LEU:HD23	2:B:777:LEU:HA	1.94	0.40
2:D:635:PHE:CD2	2:D:676:LEU:HD22	2.56	0.40
5:D:802:PEG:H41	5:D:802:PEG:H22	1.79	0.40
2:B:731:TYR:HB2	2:B:738:VAL:HG11	2.03	0.40
1:C:123:GLU:HA	1:C:127:LYS:O	2.21	0.40
2:D:582:ARG:NH1	2:D:630:LEU:CD1	2.85	0.40
2:B:681:ARG:HE	2:B:689:GLU:HG2	1.86	0.40
2:D:582:ARG:NH1	2:D:630:LEU:HD11	2.37	0.40
2:D:702:LYS:HD2	5:D:802:PEG:H41	2.04	0.40
2:D:740:ILE:HG23	2:D:789:PRO:HB3	2.03	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	181/192 (94%)	174 (96%)	6 (3%)	1 (1%)	25 62
1	C	186/192 (97%)	178 (96%)	7 (4%)	1 (0%)	29 66
2	B	299/314 (95%)	278 (93%)	18 (6%)	3 (1%)	15 52
2	D	297/314 (95%)	273 (92%)	21 (7%)	3 (1%)	15 52
3	E	5/14 (36%)	3 (60%)	2 (40%)	0	100 100
3	F	4/14 (29%)	2 (50%)	1 (25%)	1 (25%)	0 0
All	All	972/1040 (94%)	908 (93%)	55 (6%)	9 (1%)	17 54

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	158	SER
2	D	782	GLU
1	A	156	GLN
2	D	575	GLU
2	D	789	PRO
2	B	488	GLN
3	F	1333	ASP
2	B	514	ARG
2	B	783	SER

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	161/168 (96%)	156 (97%)	5 (3%)	40	70
1	C	165/168 (98%)	158 (96%)	7 (4%)	30	61
2	B	262/273 (96%)	257 (98%)	5 (2%)	57	80
2	D	260/273 (95%)	247 (95%)	13 (5%)	24	56
3	E	6/11 (54%)	6 (100%)	0	100	100
3	F	5/11 (46%)	5 (100%)	0	100	100
All	All	859/904 (95%)	829 (96%)	30 (4%)	36	67

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	65	GLU
1	A	98	SER
1	A	152	LEU
1	A	171	ASP
2	B	489	SER
2	B	504	ASP
2	B	612	SER
2	B	761	GLU
2	B	769	HIS
1	C	16	ASN
1	C	41	CYS
1	C	48	TYR
1	C	55	ASP
1	C	103	GLN
1	C	139	TYR
1	C	181	LYS
2	D	498	LEU
2	D	505	GLN
2	D	511	ASN
2	D	552	LYS
2	D	561	PHE
2	D	573	LYS
2	D	582	ARG
2	D	584	PHE
2	D	637	ARG
2	D	646	HIS
2	D	726	ARG
2	D	762	GLU
2	D	769	HIS

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

Mol	Chain	Res	Type
1	A	10	HIS
2	B	516	HIS
2	B	708	ASN
2	B	716	GLN
1	C	86	HIS
1	C	115	HIS
1	C	131	ASN

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

5 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	$\#\|Z\| > 2$
4	GOL	B	802	-	5,5,5	0.92	0	5,5,5	1.03	0
5	PEG	D	802	-	6,6,6	0.12	0	5,5,5	0.08	0
6	ACT	D	801	-	3,3,3	1.31	0	3,3,3	1.52	0
4	GOL	B	801	-	5,5,5	0.97	0	5,5,5	0.95	0
5	PEG	C	201	-	6,6,6	0.13	0	5,5,5	0.09	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
4	GOL	B	802	-	-	2/4/4/4	-
5	PEG	D	802	-	-	3/4/4/4	-
5	PEG	C	201	-	-	2/4/4/4	-
4	GOL	B	801	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801	GOL	O1-C1-C2-C3
4	B	802	GOL	O1-C1-C2-C3
5	D	802	PEG	O1-C1-C2-O2
4	B	801	GOL	C1-C2-C3-O3
4	B	801	GOL	O1-C1-C2-O2
4	B	802	GOL	O1-C1-C2-O2
4	B	801	GOL	O2-C2-C3-O3
5	D	802	PEG	C4-C3-O2-C2
5	C	201	PEG	C4-C3-O2-C2
5	C	201	PEG	C1-C2-O2-C3
5	D	802	PEG	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	802	PEG	3	0
5	C	201	PEG	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	183/192 (95%)	0.28	3 (1%) 72 69	36, 73, 111, 164	0
1	C	188/192 (97%)	0.61	14 (7%) 14 17	51, 88, 127, 181	0
2	B	301/314 (95%)	0.12	4 (1%) 77 73	37, 75, 143, 210	0
2	D	299/314 (95%)	0.08	7 (2%) 60 58	40, 77, 140, 182	2 (0%)
3	E	7/14 (50%)	1.48	3 (42%) 0 0	115, 124, 155, 215	0
3	F	6/14 (42%)	0.99	1 (16%) 1 2	110, 129, 165, 185	0
All	All	984/1040 (94%)	0.25	32 (3%) 46 44	36, 79, 138, 215	2 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	505	GLN	3.9
2	D	785	GLU	3.9
3	E	1331	PHE	3.7
2	D	784	PRO	3.4
1	C	54	GLY	3.1
2	B	519	ALA	3.0
1	C	31	ILE	3.0
3	E	1332	ASP	2.9
1	C	180	LYS	2.9
1	C	107	ASP	2.9
1	A	156	GLN	2.8
1	C	49	LEU	2.8
2	B	518	GLY	2.8
2	B	514	ARG	2.8
2	B	549	MET	2.7
1	C	51	THR	2.6
1	C	56	VAL	2.6
1	C	34	ILE	2.5
2	D	501	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	759	SER	2.4
1	A	78	GLY	2.4
2	D	783	SER	2.4
1	C	159	THR	2.4
1	C	165	TYR	2.4
2	D	522	ASN	2.3
3	E	1336	ASN	2.2
1	C	182	SER	2.2
3	F	1335	LEU	2.1
1	C	124	HIS	2.1
1	A	40	LEU	2.1
1	C	26	LEU	2.0
1	C	133	GLY	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
4	GOL	B	801	6/6	0.75	0.35	76,93,98,117	0
5	PEG	D	802	7/7	0.78	0.36	67,78,83,92	0
5	PEG	C	201	7/7	0.83	0.28	77,95,102,104	0
6	ACT	D	801	4/4	0.89	0.49	71,91,95,100	0
4	GOL	B	802	6/6	0.91	0.25	57,64,76,85	0

6.5 Other polymers (i)

There are no such residues in this entry.