



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 13, 2022 – 10:04 AM EDT

PDB ID : 7SA1
Title : LRR-F-Box plant ubiquitin ligase
Authors : Palayam, M.; Shabek, N.
Deposited on : 2021-09-21
Resolution : 3.21 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 : 2.27
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) : 2.27

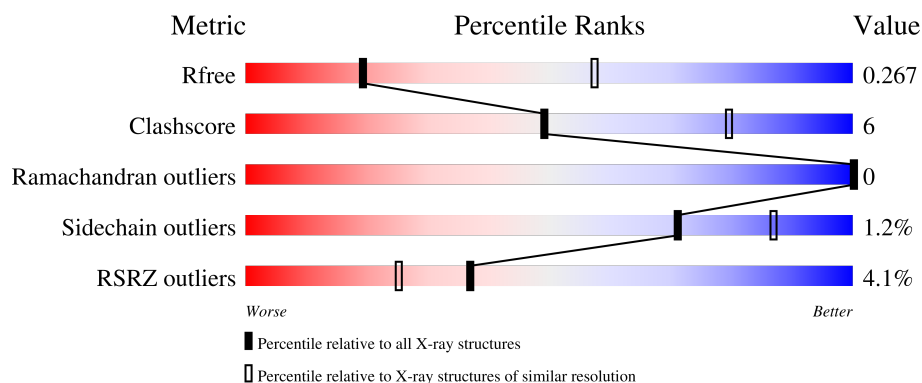
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	160	 6% 68% 8% 24%
1	C	160	 8% 68% 9% 22%
2	B	688	 2% 79% 12% 9%
2	D	688	 3% 76% 14% 9%

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
4	CIT	D	801	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11728 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 SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			978	621	159	194	4			
1	C	124	Total	C	N	O	S	0	0	0
			992	629	161	198	4			

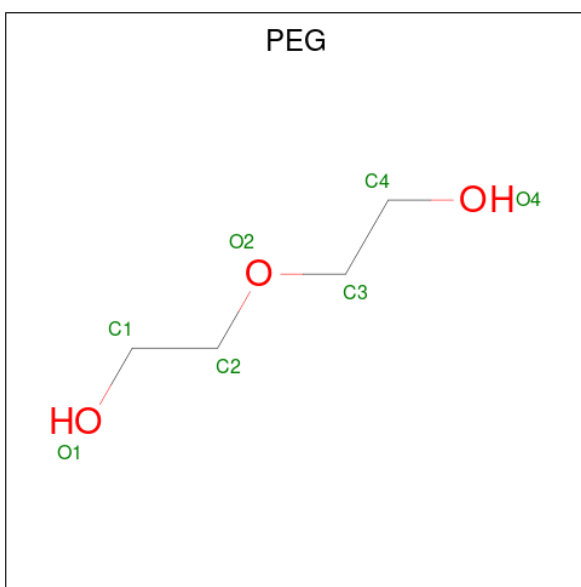
- Molecule 2 is a protein called F-box/LRR-repeat MAX2 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	624	Total	C	N	O	S	0	0	0
			4843	3081	849	883	30			
2	D	624	Total	C	N	O	S	0	0	0
			4843	3081	849	883	30			

There are 2 discrepancies between the modelled and reference sequences:

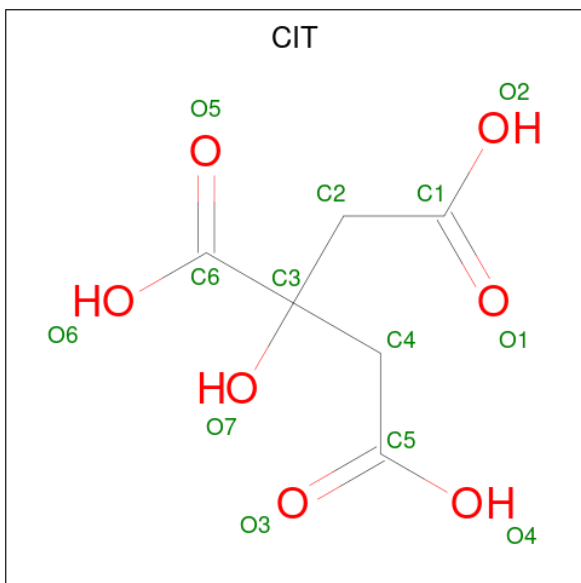
Chain	Residue	Modelled	Actual	Comment	Reference
B	720	LYS	ASP	engineered mutation	UNP Q5VMP0
D	720	LYS	ASP	engineered mutation	UNP Q5VMP0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



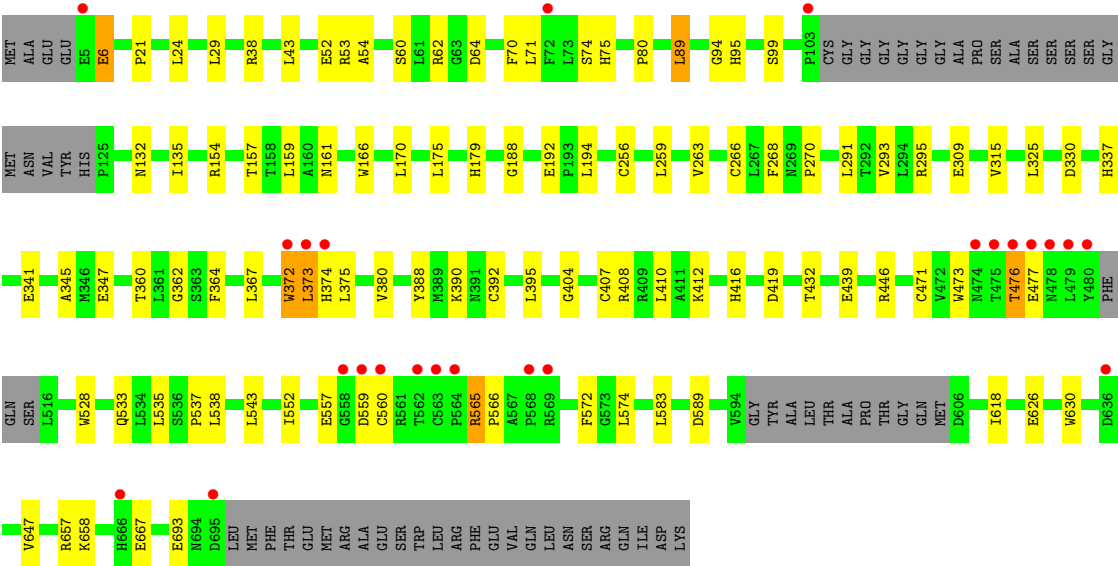
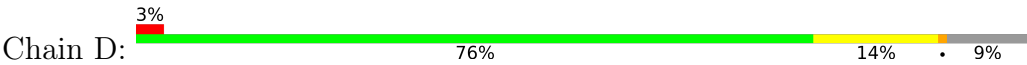
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	11	Total	O	0	0
			11	11		
5	C	1	Total	O	0	0
			1	1		
5	D	6	Total	O	0	0
			6	6		



● Molecule 2: F-box/LRR-repeat MAX2 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	231.93Å 79.41Å 150.59Å 90.00° 127.98° 90.00°	Depositor
Resolution (Å)	48.90 – 3.21 48.90 – 3.21	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.90-3.21) 87.6 (48.90-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.208 , 0.264 0.211 , 0.267	Depositor DCC
R_{free} test set	1986 reflections (5.73%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.136 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11728	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, CIT

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	0.29	0/990	0.39	0/1337
1	C	0.22	0/1004	0.36	0/1356
2	B	0.29	0/4956	0.45	0/6745
2	D	0.30	0/4956	0.44	0/6745
All	All	0.29	0/11906	0.43	0/16183

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	978	0	974	12	0
1	C	992	0	985	18	0
2	B	4843	0	4853	52	0
2	D	4843	0	4853	63	0
3	A	7	0	10	0	0
3	B	14	0	20	0	0
3	C	7	0	10	0	0
4	B	13	0	5	3	0
4	D	13	0	5	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	11	0	0	0	0
5	C	1	0	0	0	0
5	D	6	0	0	0	0
All	All	11728	0	11715	139	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 (139) 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:B:375:LEU:O	2:B:380:VAL:HG23	1.75	0.87
2:B:179:HIS:HD2	2:B:693:GLU:HG3	1.50	0.77
2:D:657:ARG:HH12	4:D:801:CIT:H22	1.49	0.76
2:D:372:TRP:H	2:D:372:TRP:HE3	1.34	0.73
2:B:375:LEU:O	2:B:380:VAL:CG2	2.36	0.72
2:B:419:ASP:HB3	2:B:446:ARG:HE	1.52	0.72
1:C:28:THR:HG23	1:C:109:ASN:HB2	1.74	0.70
1:C:6:ILE:HG13	1:C:7:VAL:N	2.06	0.69
2:D:179:HIS:HD2	2:D:693:GLU:HG3	1.59	0.67
2:B:565:ARG:HH21	2:B:609:LEU:HB3	1.62	0.63
1:C:6:ILE:HG13	1:C:7:VAL:H	1.65	0.61
1:C:6:ILE:HG23	1:C:20:GLU:HA	1.81	0.61
2:B:478:ASN:HB3	2:B:540:SER:HB2	1.81	0.61
2:D:419:ASP:HB3	2:D:446:ARG:HE	1.66	0.61
2:D:404:GLY:O	2:D:408:ARG:NH1	2.34	0.60
2:B:375:LEU:HD21	2:B:405:ARG:HB2	1.84	0.59
2:D:565:ARG:CZ	2:D:566:PRO:HD2	2.33	0.58
2:D:157:THR:O	2:D:161:ASN:ND2	2.35	0.58
2:B:266:CYS:HB3	2:B:276:VAL:HG21	1.87	0.57
2:B:475:THR:HG22	2:B:475:THR:O	2.05	0.56
2:B:538:LEU:HD11	2:B:543:LEU:HD12	1.87	0.56
1:A:130:PRO:HD3	2:B:40:ARG:HG2	1.88	0.55
2:D:21:PRO:HD2	2:D:24:LEU:HD12	1.88	0.55
2:D:159:LEU:HD13	2:D:194:LEU:HG	1.90	0.54
2:B:431:PHE:HE2	2:D:6:GLU:O	1.91	0.54
2:D:626:GLU:HG3	2:D:658:LYS:HB2	1.89	0.54
2:B:263:VAL:HG22	2:B:295:ARG:HB2	1.89	0.54
2:B:159:LEU:HD13	2:B:194:LEU:HG	1.89	0.54
2:D:263:VAL:HG22	2:D:295:ARG:HB2	1.89	0.53
2:D:538:LEU:HD11	2:D:543:LEU:HD12	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:471:CYS:O	2:D:533:GLN:NE2	2.34	0.53
2:D:291:LEU:HB2	2:D:325:LEU:HD22	1.90	0.53
1:A:134:ARG:HG3	1:A:139:ILE:HB	1.91	0.53
2:B:471:CYS:O	2:B:533:GLN:NE2	2.29	0.53
2:D:159:LEU:HD21	2:D:175:LEU:HD21	1.89	0.52
2:D:528:TRP:HE3	2:D:557:GLU:OE1	1.92	0.52
2:D:574:LEU:HD23	2:D:618:ILE:HB	1.91	0.52
2:B:309:GLU:OE1	2:B:309:GLU:N	2.42	0.52
4:D:801:CIT:O2	4:D:801:CIT:O7	2.27	0.51
2:D:589:ASP:HA	2:D:630:TRP:HB2	1.91	0.51
1:A:139:ILE:HG23	2:B:18:LEU:HD11	1.93	0.51
2:D:94:GLY:O	2:D:154:ARG:NH1	2.40	0.51
2:D:657:ARG:NH1	4:D:801:CIT:H22	2.23	0.50
2:B:29:LEU:O	2:B:38:ARG:NH1	2.44	0.50
2:D:54:ALA:HA	2:D:80:PRO:HD2	1.93	0.50
2:B:52:GLU:OE1	2:B:53:ARG:NH1	2.45	0.50
2:B:54:ALA:HA	2:B:80:PRO:HD2	1.94	0.50
2:D:407:CYS:HB3	2:D:410:LEU:HG	1.93	0.50
2:D:364:PHE:HB3	2:D:367:LEU:HD21	1.93	0.49
2:B:163:THR:N	2:B:164:PRO:HD2	2.27	0.49
2:D:647:VAL:HG11	2:D:667:GLU:HG3	1.94	0.49
1:C:6:ILE:CG1	1:C:7:VAL:H	2.21	0.49
2:B:574:LEU:HD23	2:B:618:ILE:HB	1.94	0.49
2:B:374:HIS:O	2:B:375:LEU:HG	2.13	0.48
2:D:60:SER:OG	2:D:89:LEU:CD1	2.61	0.48
1:C:6:ILE:CG2	1:C:20:GLU:HB2	2.44	0.48
2:D:657:ARG:HH22	4:D:801:CIT:C2	2.27	0.48
1:A:58:TYR:HA	1:A:86:TRP:HH2	1.78	0.48
2:B:676:ILE:HD12	2:B:679:LEU:HD22	1.95	0.48
2:B:266:CYS:HB2	2:B:268:PHE:CE2	2.49	0.47
2:D:392:CYS:SG	2:D:395:LEU:HB2	2.54	0.47
1:A:7:VAL:HG12	1:A:7:VAL:O	2.14	0.47
2:B:647:VAL:HG11	2:B:667:GLU:HG3	1.95	0.47
2:B:315:VAL:HG11	2:B:341:GLU:HG3	1.96	0.47
2:D:360:THR:HG23	2:D:388:TYR:HB3	1.95	0.47
2:B:565:ARG:NH1	2:B:566:PRO:O	2.47	0.47
1:C:6:ILE:HG23	1:C:20:GLU:CB	2.45	0.47
2:B:535:LEU:HB2	2:B:572:PHE:CZ	2.51	0.46
2:B:626:GLU:HG3	2:B:658:LYS:HB2	1.97	0.46
2:D:52:GLU:OE1	2:D:53:ARG:NH1	2.48	0.46
1:A:130:PRO:O	1:A:134:ARG:HD3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:476:THR:HG23	2:D:477:GLU:HG3	1.98	0.46
1:A:61:ARG:HG2	1:A:86:TRP:CE3	2.51	0.46
2:D:99:SER:O	2:D:132:ASN:ND2	2.42	0.46
2:D:657:ARG:HH22	4:D:801:CIT:H22	1.80	0.46
2:B:392:CYS:SG	2:B:395:LEU:HB2	2.56	0.46
1:A:6:ILE:HG22	1:A:6:ILE:O	2.16	0.46
2:B:82:LEU:HD22	2:B:143:PHE:HB3	1.97	0.46
1:C:6:ILE:HG23	1:C:20:GLU:CA	2.45	0.45
1:C:156:GLN:HG3	2:D:62:ARG:HH12	1.81	0.45
2:B:657:ARG:NH2	2:B:680:ARG:HD2	2.30	0.45
2:B:40:ARG:HA	2:B:43:LEU:HD12	1.98	0.45
1:C:130:PRO:O	1:C:134:ARG:HD3	2.16	0.45
2:B:589:ASP:HA	2:B:630:TRP:HB2	1.97	0.45
1:C:157:TRP:CH2	2:D:70:PHE:HB2	2.51	0.45
2:B:291:LEU:HB2	2:B:325:LEU:HD22	1.98	0.45
2:D:374:HIS:CD2	2:D:375:LEU:HG	2.52	0.45
2:D:412:LYS:HG2	2:D:439:GLU:HB2	1.98	0.45
1:C:61:ARG:HG2	1:C:86:TRP:CE3	2.52	0.44
2:D:315:VAL:HG11	2:D:341:GLU:HG3	1.99	0.44
1:A:146:GLU:N	1:A:146:GLU:OE1	2.50	0.44
2:B:374:HIS:HB3	2:B:375:LEU:H	1.55	0.44
1:A:157:TRP:CH2	2:B:70:PHE:HB2	2.52	0.44
2:B:415:ILE:HD11	2:B:426:ILE:HD11	2.00	0.44
2:D:362:GLY:HA2	2:D:390:LYS:HB2	1.98	0.44
2:B:390:LYS:HG2	2:B:416:HIS:HB3	2.00	0.44
2:D:60:SER:OG	2:D:89:LEU:HD12	2.18	0.44
2:D:71:LEU:HD21	2:D:135:ILE:HG12	2.00	0.44
2:B:315:VAL:HG23	2:B:345:ALA:HB2	2.00	0.44
2:B:410:LEU:HD23	2:B:410:LEU:HA	1.83	0.44
2:D:408:ARG:NH2	2:D:432:THR:O	2.51	0.44
4:B:803:CIT:O1	4:B:803:CIT:O7	2.33	0.43
1:C:58:TYR:HA	1:C:86:TRP:HH2	1.83	0.43
2:B:657:ARG:HH22	4:B:803:CIT:H42	1.81	0.43
2:D:270:PRO:HD2	2:D:337:HIS:CE1	2.54	0.43
1:C:152:ARG:HG2	2:D:43:LEU:HD21	1.99	0.43
2:D:170:LEU:HD12	2:D:170:LEU:HA	1.86	0.43
2:B:39:HIS:CD2	2:B:56:ARG:HH22	2.37	0.43
2:B:687:ASP:OD1	2:B:687:ASP:N	2.47	0.43
2:B:360:THR:HG23	2:B:388:TYR:HB3	2.00	0.43
4:B:803:CIT:O7	4:B:803:CIT:O4	2.35	0.43
2:D:373:LEU:HB3	2:D:374:HIS:H	1.63	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:VAL:HG22	2:B:330:ASP:HB3	2.00	0.43
1:A:28:THR:HG23	1:A:109:ASN:HB2	2.01	0.43
2:D:552:ILE:HG22	2:D:583:LEU:HD11	2.01	0.43
1:C:157:TRP:HZ3	2:D:64:ASP:H	1.67	0.42
2:D:256:CYS:HB2	2:D:259:LEU:HG	2.01	0.42
2:D:347:GLU:HG2	2:D:380:VAL:HG21	2.02	0.42
2:D:29:LEU:O	2:D:38:ARG:NH1	2.51	0.42
2:D:315:VAL:HG23	2:D:345:ALA:HB2	2.02	0.42
2:D:410:LEU:HD23	2:D:410:LEU:HA	1.83	0.42
1:C:134:ARG:HA	1:C:139:ILE:HB	2.01	0.42
2:D:535:LEU:HB2	2:D:572:PHE:CZ	2.54	0.42
2:B:478:ASN:HD22	2:B:480:TYR:HD2	1.68	0.42
1:C:61:ARG:HG2	1:C:86:TRP:CD2	2.55	0.42
2:D:74:SER:OG	2:D:75:HIS:N	2.53	0.41
2:D:309:GLU:OE1	2:D:309:GLU:N	2.49	0.41
2:D:528:TRP:CE3	2:D:557:GLU:OE1	2.72	0.41
1:C:27:GLN:HB2	1:C:109:ASN:HB3	2.02	0.41
2:D:293:VAL:HG22	2:D:330:ASP:HB3	2.03	0.41
2:B:179:HIS:CD2	2:B:693:GLU:HG3	2.41	0.41
2:D:473:TRP:CD2	2:D:537:PRO:HB2	2.56	0.41
1:A:134:ARG:HD2	2:B:44:ALA:HA	2.03	0.41
2:B:523:ARG:NH1	2:B:550:GLU:OE1	2.54	0.41
2:B:375:LEU:O	2:B:380:VAL:HG22	2.19	0.40
2:D:188:GLY:O	2:D:192:GLU:HG3	2.22	0.40
2:D:390:LYS:HG2	2:D:416:HIS:HB3	2.02	0.40
2:D:266:CYS:HB2	2:D:268:PHE:CE2	2.57	0.40
2:D:166:TRP:O	2:D:170:LEU:HB2	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	114/160 (71%)	108 (95%)	6 (5%)	0	100	100
1	C	116/160 (72%)	113 (97%)	3 (3%)	0	100	100
2	B	616/688 (90%)	576 (94%)	40 (6%)	0	100	100
2	D	616/688 (90%)	582 (94%)	34 (6%)	0	100	100
All	All	1462/1696 (86%)	1379 (94%)	83 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/137 (80%)	108 (99%)	1 (1%)	78	90
1	C	110/137 (80%)	110 (100%)	0	100	100
2	B	526/575 (92%)	521 (99%)	5 (1%)	76	89
2	D	526/575 (92%)	517 (98%)	9 (2%)	60	82
All	All	1271/1424 (89%)	1256 (99%)	15 (1%)	71	87

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
2	B	90	VAL
2	B	369	LYS
2	B	374	HIS
2	B	474	ASN
2	B	636	ASP
2	D	6	GLU
2	D	89	LEU
2	D	95	HIS
2	D	372	TRP
2	D	373	LEU
2	D	476	THR
2	D	559	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	560	CYS
2	D	565	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
2	B	131	GLN
1	C	109	ASN
2	D	131	GLN
2	D	337	HIS
2	D	374	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
3	PEG	A	801	-	6,6,6	0.50	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	B	802	-	6,6,6	0.48	0	5,5,5	0.33	0
3	PEG	B	801	-	6,6,6	0.49	0	5,5,5	0.28	0
4	CIT	B	803	-	3,12,12	1.36	0	3,17,17	2.41	2 (66%)
3	PEG	C	201	-	6,6,6	0.49	0	5,5,5	0.26	0
4	CIT	D	801	-	3,12,12	0.70	0	3,17,17	0.27	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
3	PEG	A	801	-	-	2/4/4/4	-
3	PEG	B	802	-	-	2/4/4/4	-
3	PEG	B	801	-	-	3/4/4/4	-
4	CIT	B	803	-	-	3/6/16/16	-
3	PEG	C	201	-	-	1/4/4/4	-
4	CIT	D	801	-	-	3/6/16/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	CIT	C3-C4-C5	-2.99	110.20	114.98
4	B	803	CIT	C3-C2-C1	-2.91	110.33	114.98

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	801	CIT	C1-C2-C3-C6
4	D	801	CIT	C1-C2-C3-O7
3	A	801	PEG	O1-C1-C2-O2
4	D	801	CIT	C1-C2-C3-C4
3	B	801	PEG	O2-C3-C4-O4
3	A	801	PEG	C1-C2-O2-C3
3	B	801	PEG	C1-C2-O2-C3
3	B	802	PEG	O1-C1-C2-O2
3	B	802	PEG	C4-C3-O2-C2
4	B	803	CIT	C1-C2-C3-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	803	CIT	C1-C2-C3-O7
3	B	801	PEG	C4-C3-O2-C2
4	B	803	CIT	C2-C3-C4-C5
3	C	201	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	803	CIT	3	0
4	D	801	CIT	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	122/160 (76%)	0.46	10 (8%) 11 7	21, 69, 111, 145	0
1	C	124/160 (77%)	0.50	13 (10%) 6 4	25, 72, 113, 152	0
2	B	624/688 (90%)	-0.23	14 (2%) 62 49	12, 32, 83, 137	0
2	D	624/688 (90%)	-0.13	24 (3%) 40 27	14, 36, 89, 137	0
All	All	1494/1696 (88%)	-0.07	61 (4%) 37 25	12, 36, 101, 152	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	560	CYS	4.8
2	B	372	TRP	4.6
1	A	22	VAL	4.5
1	A	23	ALA	4.5
1	A	81	ASP	4.4
2	D	563	CYS	4.3
2	B	636	ASP	4.2
1	C	8	LEU	4.1
2	D	480	TYR	4.1
2	D	562	THR	4.0
1	C	82	ASP	4.0
2	D	372	TRP	3.9
2	B	374	HIS	3.6
1	A	82	ASP	3.6
1	C	29	ILE	3.5
2	D	373	LEU	3.3
2	D	476	THR	3.2
2	D	564	PRO	3.2
2	D	558	GLY	3.2
2	B	72	PHE	3.2
1	C	21	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	24	LEU	3.0
1	A	55	VAL	3.0
2	D	477	GLU	2.9
2	B	564	PRO	2.9
1	C	60	LYS	2.9
2	D	479	LEU	2.8
2	B	371	SER	2.7
1	C	22	VAL	2.7
2	D	374	HIS	2.7
2	D	559	ASP	2.6
1	C	81	ASP	2.6
2	D	72	PHE	2.5
2	D	569	ARG	2.5
1	A	29	ILE	2.5
2	B	476	THR	2.4
2	D	568	PRO	2.4
1	A	56	ILE	2.4
1	C	42	VAL	2.4
2	D	474	ASN	2.4
1	C	27	GLN	2.3
2	B	560	CYS	2.3
2	B	477	GLU	2.3
2	D	103	PRO	2.3
2	D	666	HIS	2.3
2	B	480	TYR	2.3
2	D	636	ASP	2.3
2	B	479	LEU	2.3
1	C	20	GLU	2.3
1	A	43	PRO	2.2
2	D	5	GLU	2.2
1	C	28	THR	2.2
2	D	695	ASP	2.2
1	A	24	LEU	2.1
2	B	559	ASP	2.1
2	B	9	GLU	2.1
1	A	60	LYS	2.1
1	C	9	LYS	2.1
2	B	103	PRO	2.0
2	D	478	ASN	2.0
2	D	475	THR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CIT	D	801	13/13	0.65	0.40	46,69,101,107	0
3	PEG	B	802	7/7	0.79	0.26	39,44,58,64	0
4	CIT	B	803	13/13	0.83	0.25	47,65,77,80	0
3	PEG	B	801	7/7	0.89	0.30	29,44,62,68	0
3	PEG	C	201	7/7	0.90	0.18	18,21,35,44	0
3	PEG	A	801	7/7	0.91	0.16	24,29,39,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.