Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 02:17 PM EDT

PDB ID	:	6TTK
Title	:	Crystal structure of the kelch domain of human KLHL12 in complex with DVL1 peptide
Authors	:	Chen, Z.; Williams, E.; Pike, A.C.W.; Strain-Damerell, C.; Wang, D.; Chalk, R.; Burgess-Brown, N.; Krojer, T.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Bullock, A.N.
Deposited on	:	2019-12-27
Resolution	:	2.38 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 (i) 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 (i)) were used in the production of this report:

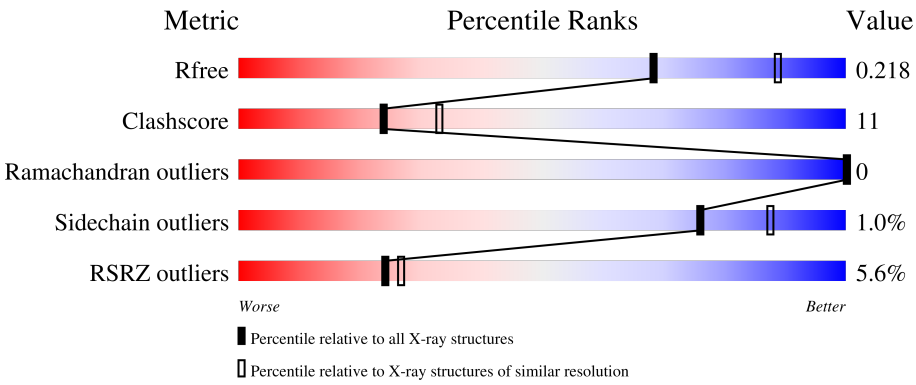
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	301	3% 75% 19% • 5%
1	B	301	4% 70% 24% • 5%
1	C	301	2% 75% 18% • 6%
1	D	301	7% 77% 18% • 5%

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Mol	Chain	Length	Quality of chain
2	E	15	27% 40% 7% 7% 47%
2	F	15	13% 27% 20% 53%
2	G	15	27% 53% 47%
2	H	15	27% 40% 13% 47%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9388 atoms, of which 6 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 Kelch-like protein 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	2143	1347	366	416	14	0	0	0
1	B	285	2142	1347	360	420	15	0	1	0
1	C	284	2143	1343	366	419	15	0	2	0
1	D	286	2124	1330	362	417	15	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	SER	-	expression tag	UNP Q53G59
B	267	SER	-	expression tag	UNP Q53G59
C	267	SER	-	expression tag	UNP Q53G59
D	267	SER	-	expression tag	UNP Q53G59

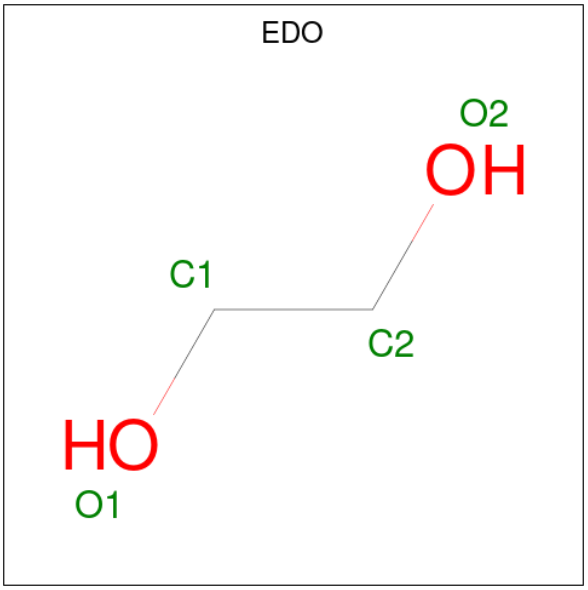
- Molecule 2 is a protein called DVL1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	F	7	37	23	7	7	0	0	0
2	G	8	47	31	8	8	0	0	0
2	H	8	45	29	8	8	0	0	0
2	E	8	47	31	8	8	0	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0
			Total	Na		
3	B	2	2	2	0	0
			Total	Na		
3	C	1	1	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	10	2	6	2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	D	1	1	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	158	158	158	0	0
			Total	O		
6	B	172	172	172	0	0

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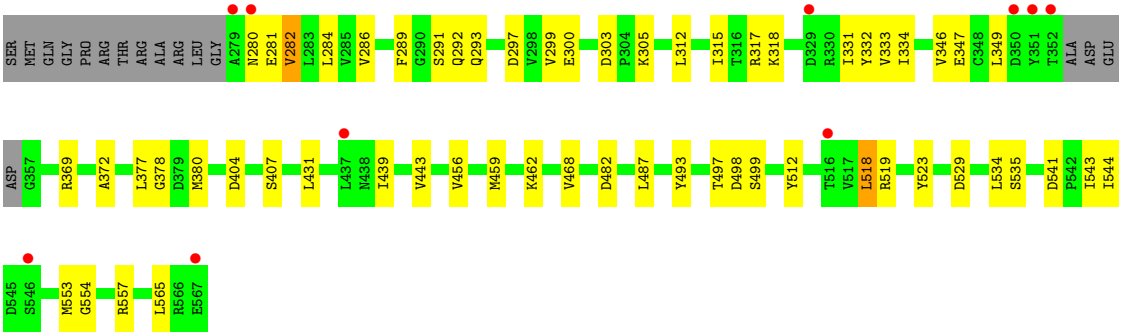
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	C	188	188	188	0	0
			Total	O		
6	D	122	122	122	0	0
			Total	O		
6	F	2	2	2	0	0
			Total	O		
6	H	1	1	1	0	0
			Total	O		
6	E	2	2	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

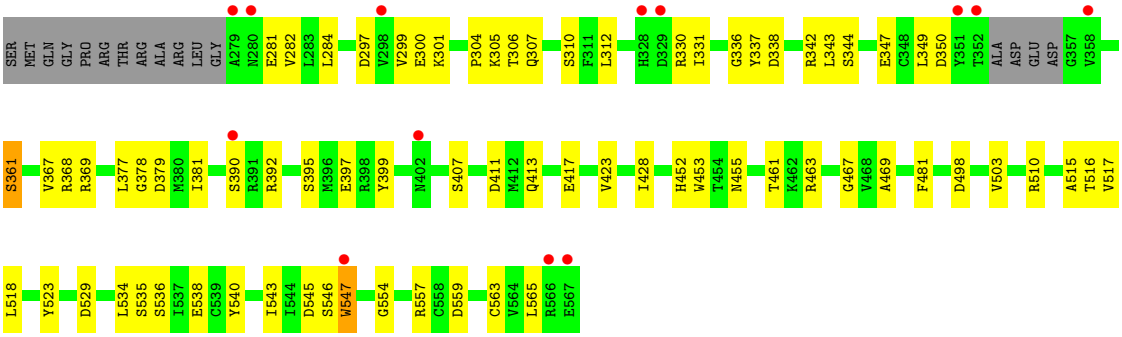
- Molecule 1: Kelch-like protein 12

Chain A:



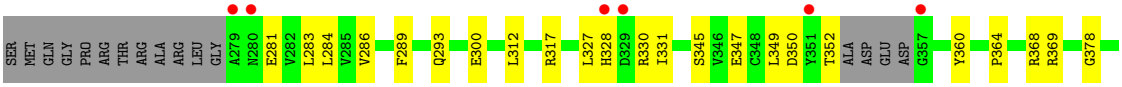
- Molecule 1: Kelch-like protein 12

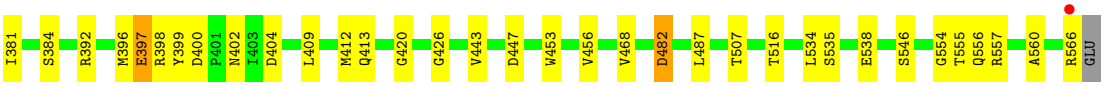
Chain B:



- Molecule 1: Kelch-like protein 12

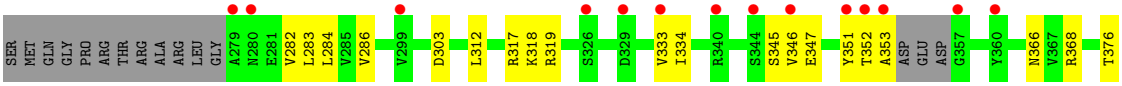
Chain C:

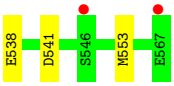




• Molecule 1: Kelch-like protein 12

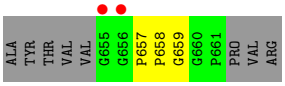
Chain D:





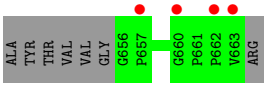
• Molecule 2: DVL1

Chain F:



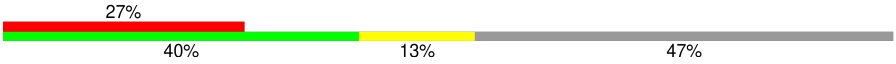
• Molecule 2: DVL1

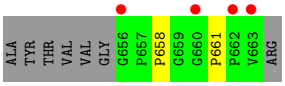
Chain G:



• Molecule 2: DVL1

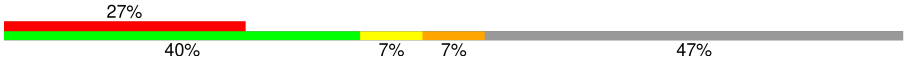
Chain H:

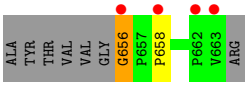




• Molecule 2: DVL1

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.22Å 73.14Å 101.84Å 90.00° 94.50° 90.00°	Depositor
Resolution (Å)	79.98 – 2.38 79.98 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.6 (79.98-2.38) 99.6 (79.98-2.38)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.225 , 0.251 0.227 , 0.218	Depositor DCC
R_{free} test set	2438 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.842	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9388	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7723e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, EDO

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	0.74	1/2189 (0.0%)	0.75	2/2982 (0.1%)
1	B	0.78	4/2191 (0.2%)	0.77	1/2984 (0.0%)
1	C	0.77	4/2192 (0.2%)	0.77	2/2987 (0.1%)
1	D	0.66	1/2172 (0.0%)	0.77	0/2962
2	E	1.68	0/50	1.93	1/70 (1.4%)
2	F	2.08	1/39 (2.6%)	2.05	1/53 (1.9%)
2	G	0.38	0/50	0.45	0/70
2	H	1.62	0/48	1.40	0/67
All	All	0.77	11/8931 (0.1%)	0.79	7/12175 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	397	GLU	CD-OE1	-9.18	1.15	1.25
1	B	547	TRP	CE3-CZ3	-7.79	1.25	1.38
1	C	397	GLU	CD-OE2	-7.68	1.17	1.25
2	F	657	PRO	N-CD	-7.61	1.37	1.47
1	B	453	TRP	CE3-CZ3	-7.57	1.25	1.38
1	D	434	TYR	CE1-CZ	-6.26	1.30	1.38
1	C	426	GLY	C-O	-5.29	1.15	1.23
1	B	453	TRP	CB-CG	-5.28	1.40	1.50
1	B	547	TRP	CD2-CE2	-5.23	1.35	1.41
1	C	345	SER	CB-OG	-5.14	1.35	1.42
1	A	282	VAL	C-O	-5.10	1.13	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	553	MET	N-CA-C	7.52	131.30	111.00
2	F	659	GLY	N-CA-C	-7.22	95.05	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	482	ASP	CB-CG-OD1	6.29	123.96	118.30
1	B	297	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	368	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	518	LEU	CA-CB-CG	5.58	128.12	115.30
2	E	656	GLY	C-N-CD	5.01	138.93	128.40

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	2143	0	2044	43	1
1	B	2142	0	2038	65	0
1	C	2143	0	2033	37	0
1	D	2124	0	1994	43	0
2	E	47	0	45	2	0
2	F	37	0	32	2	0
2	G	47	0	45	0	0
2	H	45	0	38	4	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
4	A	4	6	6	0	0
5	D	1	0	0	0	0
6	A	158	0	0	11	4
6	B	172	0	0	15	2
6	C	188	0	0	12	2
6	D	122	0	0	9	1
6	E	2	0	0	1	0
6	F	2	0	0	0	0
6	H	1	0	0	0	0
All	All	9382	6	8275	188	7

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 11.

All (188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:ASN:OD1	6:B:701:HOH:O	1.54	1.20
1:B:282:VAL:HG22	1:B:565:LEU:CD1	1.75	1.17
1:B:282:VAL:CG2	1:B:565:LEU:HD11	1.81	1.11
1:B:392:ARG:NH2	6:B:703:HOH:O	1.84	1.10
1:D:392:ARG:NH2	6:D:702:HOH:O	1.87	1.06
1:B:282:VAL:HG22	1:B:565:LEU:HD11	1.37	1.03
1:A:280:ASN:OD1	6:A:701:HOH:O	1.79	0.97
1:B:347:GLU:HB3	6:B:710:HOH:O	1.63	0.95
1:D:347:GLU:OE1	6:D:701:HOH:O	1.81	0.94
1:B:413:GLN:NE2	6:B:706:HOH:O	2.02	0.93
1:A:305:LYS:HE3	6:A:733:HOH:O	1.73	0.87
1:B:379:ASP:OD2	6:B:704:HOH:O	1.95	0.83
1:B:282:VAL:HG21	1:B:565:LEU:HD11	1.61	0.82
1:B:282:VAL:CG2	1:B:565:LEU:CD1	2.49	0.78
1:B:452:HIS:NE2	6:B:711:HOH:O	2.16	0.78
1:B:395:SER:HA	1:B:411:ASP:OD2	1.85	0.77
1:A:286:VAL:HG13	1:A:299:VAL:HG22	1.68	0.76
1:B:565:LEU:HD12	1:B:565:LEU:O	1.88	0.73
1:B:281:GLU:OE2	6:B:707:HOH:O	2.07	0.73
1:B:407:SER:OG	6:B:702:HOH:O	1.78	0.72
1:C:317:ARG:NH2	6:C:702:HOH:O	2.23	0.71
1:B:498:ASP:OD2	6:B:708:HOH:O	2.08	0.71
1:C:378:GLY:HA3	6:C:703:HOH:O	1.91	0.71
1:A:297:ASP:HB3	1:A:318:LYS:HG2	1.71	0.70
1:A:439:ILE:HG22	1:A:462:LYS:HB3	1.71	0.70
1:C:447:ASP:OD2	6:C:701:HOH:O	2.08	0.70
1:B:282:VAL:HG22	1:B:565:LEU:HD12	1.73	0.69
1:A:281:GLU:OE2	1:A:519:ARG:HG2	1.91	0.69
1:D:368:ARG:O	6:D:704:HOH:O	2.11	0.69
1:A:292:GLN:HG3	6:A:774:HOH:O	1.93	0.69
1:B:361:SER:HB2	6:B:790:HOH:O	1.92	0.68
1:C:281:GLU:HG2	1:C:566:ARG:HG3	1.73	0.68
1:C:330:ARG:HD2	1:C:350:ASP:OD1	1.93	0.68
1:D:553:MET:HG2	6:D:740:HOH:O	1.92	0.68
1:A:292:GLN:CG	6:A:774:HOH:O	2.42	0.67
1:B:347:GLU:CB	6:B:710:HOH:O	2.28	0.67
1:C:328:HIS:HD2	6:C:854:HOH:O	1.76	0.67
1:A:512:TYR:OH	2:E:658:PRO:O	2.06	0.67
1:B:347:GLU:OE1	6:B:710:HOH:O	2.12	0.67
1:B:369:ARG:NH2	1:B:397:GLU:OE2	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:SER:HB2	1:B:554:GLY:O	1.96	0.65
1:C:399:TYR:OH	1:C:404:ASP:OD1	2.10	0.65
1:D:516:THR:HG22	1:D:523:TYR:HB2	1.77	0.65
1:B:543:ILE:HD13	6:B:742:HOH:O	1.98	0.64
1:B:342:ARG:O	1:B:368:ARG:HD3	1.98	0.63
1:D:351:TYR:O	1:D:353:ALA:N	2.32	0.63
1:D:351:TYR:C	1:D:353:ALA:N	2.48	0.62
1:B:395:SER:CA	1:B:411:ASP:OD2	2.47	0.62
1:B:540:TYR:HB2	1:B:547:TRP:CZ2	2.36	0.61
1:D:529:ASP:HB3	1:D:534:LEU:HD21	1.82	0.61
1:D:521:ARG:NH2	1:D:541:ASP:OD2	2.34	0.60
1:D:393:HIS:CD2	6:D:704:HOH:O	2.53	0.60
1:C:468:VAL:HG22	6:C:818:HOH:O	2.01	0.60
1:D:351:TYR:C	1:D:353:ALA:H	2.05	0.59
1:D:512:TYR:OH	2:H:658:PRO:O	2.17	0.59
1:A:529:ASP:HB3	1:A:534:LEU:HD21	1.84	0.59
1:C:283:LEU:HD22	1:C:516:THR:HG21	1.86	0.58
1:B:344:SER:HB3	1:B:368:ARG:HG2	1.86	0.58
1:D:283:LEU:HD21	1:D:516:THR:HG21	1.85	0.57
1:C:347:GLU:HB3	6:C:716:HOH:O	2.05	0.57
1:B:367:VAL:HG12	1:B:369:ARG:HG2	1.86	0.57
1:A:482:ASP:HB3	1:A:487:LEU:HD11	1.87	0.57
1:A:518:LEU:HD13	1:A:519:ARG:HG3	1.86	0.57
1:D:409:LEU:HD23	1:D:446:TYR:OH	2.04	0.56
1:B:498:ASP:CG	1:B:498:ASP:O	2.44	0.56
1:D:416:ARG:HH21	1:D:444:GLU:HG3	1.70	0.56
1:A:334:ILE:HA	1:A:346:VAL:HG22	1.87	0.56
1:B:282:VAL:HG22	1:B:565:LEU:CG	2.33	0.55
1:C:300:GLU:OE1	1:C:555[A]:THR:HG23	2.06	0.55
1:D:376:THR:O	1:D:423:VAL:HG21	2.06	0.55
1:B:540:TYR:HB2	1:B:547:TRP:CE2	2.41	0.55
1:D:318:LYS:HE2	6:D:805:HOH:O	2.07	0.55
1:A:331:ILE:HD12	1:A:349:LEU:HD23	1.89	0.54
1:C:289:PHE:CZ	1:C:293:GLN:HA	2.42	0.54
1:C:443:VAL:HB	1:C:456:VAL:HB	1.89	0.54
1:C:331:ILE:HD12	1:C:349:LEU:HD23	1.89	0.53
1:D:510:ARG:NH2	1:D:538:GLU:HG2	2.24	0.53
1:D:286:VAL:HG21	1:D:333:VAL:HG21	1.90	0.53
1:D:400:ASP:OD2	6:D:706:HOH:O	2.18	0.53
1:B:342:ARG:HD3	6:B:741:HOH:O	2.08	0.52
1:D:427:VAL:HG11	1:D:445:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:ILE:HA	1:D:346:VAL:HG22	1.92	0.52
1:D:351:TYR:O	1:D:352:THR:C	2.47	0.52
2:E:656:GLY:N	6:E:701:HOH:O	2.42	0.52
1:A:284:LEU:HD11	1:A:312:LEU:HD22	1.91	0.52
1:B:392:ARG:NE	1:B:417:GLU:OE2	2.44	0.51
1:B:330:ARG:HG2	1:B:350:ASP:OD1	2.10	0.51
1:B:481:PHE:CD2	2:F:658:PRO:HB2	2.45	0.51
1:C:420:GLY:N	6:C:706:HOH:O	2.31	0.50
1:B:304:PRO:HG3	1:B:518:LEU:HD22	1.93	0.50
1:B:300:GLU:HB2	1:B:557:ARG:NH2	2.26	0.50
1:A:284:LEU:HD22	1:A:565:LEU:HD11	1.94	0.49
1:C:392:ARG:NH2	6:C:714:HOH:O	2.42	0.49
1:C:369:ARG:HH21	1:C:397:GLU:HG2	1.77	0.49
1:A:289:PHE:O	1:A:557:ARG:HA	2.12	0.49
1:B:529:ASP:HB3	1:B:534:LEU:HD21	1.95	0.49
1:B:413:GLN:HA	1:C:413:GLN:HE22	1.77	0.49
1:B:331:ILE:HD12	1:B:349:LEU:HD23	1.94	0.48
1:B:481:PHE:HD2	2:F:658:PRO:HB2	1.78	0.48
1:A:281:GLU:HB2	1:A:518:LEU:HD22	1.94	0.48
1:B:299:VAL:HG12	1:B:312:LEU:HB2	1.96	0.48
1:D:528:TYR:CG	2:H:661:PRO:HG3	2.49	0.48
1:B:423:VAL:HG22	1:B:428:ILE:HG12	1.96	0.48
1:A:286:VAL:HG11	1:A:333:VAL:HG21	1.96	0.48
1:B:395:SER:CB	1:B:411:ASP:OD2	2.62	0.48
1:B:282:VAL:CG2	1:B:565:LEU:CG	2.90	0.48
1:D:481:PHE:HB2	1:D:511[A]:CYS:SG	2.54	0.48
1:A:332:TYR:OH	6:A:702:HOH:O	2.15	0.47
1:D:470:LEU:HA	1:D:474:HIS:O	2.13	0.47
1:D:319:ARG:NH2	1:D:345:SER:OG	2.38	0.47
1:C:352:THR:HA	6:C:737:HOH:O	2.15	0.47
1:D:469:ALA:HB3	1:D:522:LEU:CD1	2.44	0.47
1:A:282:VAL:HG12	1:A:303:ASP:HA	1.95	0.47
1:C:300:GLU:CD	1:C:555[A]:THR:HG23	2.35	0.47
1:C:364:PRO:HG2	6:C:785:HOH:O	2.14	0.47
1:A:431:LEU:HB3	1:A:459:MET:CE	2.44	0.47
1:A:443:VAL:HB	1:A:456:VAL:HG22	1.96	0.47
1:C:420:GLY:HA3	1:C:468:VAL:HG21	1.95	0.47
1:D:513:VAL:HG23	1:D:525:ILE:O	2.15	0.47
1:C:412:MET:HG2	1:C:453:TRP:CE2	2.49	0.47
1:A:543:ILE:HG23	1:A:544:ILE:HG23	1.98	0.46
1:D:409:LEU:HD12	1:D:409:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:SER:HB2	1:A:554:GLY:O	2.16	0.46
1:B:516:THR:HG22	1:B:523:TYR:HB2	1.97	0.46
1:C:289:PHE:O	1:C:557:ARG:HA	2.15	0.46
1:D:282:VAL:HG12	1:D:303:ASP:HA	1.96	0.46
1:B:377:LEU:HD12	1:B:378:GLY:H	1.80	0.46
1:A:541:ASP:HB3	1:A:544:ILE:HG12	1.98	0.46
1:A:518:LEU:HB3	1:A:523:TYR:CE1	2.51	0.46
1:A:377:LEU:HD12	1:A:378:GLY:H	1.81	0.46
1:A:404:ASP:HB3	6:A:706:HOH:O	2.17	0.45
1:A:407:SER:OG	6:A:703:HOH:O	2.19	0.45
1:C:286:VAL:O	1:C:560:ALA:HB1	2.17	0.45
1:A:284:LEU:HD21	1:A:331:ILE:HD13	1.99	0.45
1:D:284:LEU:HD11	1:D:312:LEU:HD22	1.99	0.44
1:B:336:GLY:O	1:B:343:LEU:N	2.47	0.44
1:B:381:ILE:HB	1:B:399:TYR:HB3	1.98	0.44
1:B:301:LYS:HB2	1:B:312:LEU:CD1	2.47	0.44
1:C:327:LEU:O	1:C:330:ARG:HB2	2.17	0.44
1:D:493:TYR:OH	1:D:498:ASP:HA	2.17	0.44
1:B:503:VAL:HA	6:B:802:HOH:O	2.18	0.43
1:B:281:GLU:O	1:B:518:LEU:HD11	2.18	0.43
1:B:284:LEU:HD23	1:B:563:CYS:SG	2.57	0.43
1:C:400:ASP:OD1	1:C:402:ASN:HB2	2.17	0.43
1:A:468:VAL:HG22	6:A:832:HOH:O	2.18	0.43
1:B:306:THR:O	1:B:307:GLN:CB	2.63	0.43
1:A:519:ARG:NH1	6:A:717:HOH:O	2.51	0.43
1:C:482:ASP:HB3	1:C:487:LEU:HD11	2.00	0.43
1:C:360:TYR:HB2	6:C:743:HOH:O	2.17	0.43
1:A:293:GLN:NE2	6:A:707:HOH:O	2.32	0.43
1:D:493:TYR:HB2	1:D:500:TRP:CH2	2.54	0.43
1:C:535:SER:HB2	1:C:554:GLY:O	2.18	0.43
1:D:366:ASN:HB2	1:D:408:MET:SD	2.58	0.42
1:D:528:TYR:CD1	2:H:661:PRO:HG3	2.54	0.42
1:A:443:VAL:HB	1:A:456:VAL:CG2	2.50	0.42
1:B:337:TYR:CD1	1:B:342:ARG:HD2	2.54	0.42
1:B:510:ARG:NH1	1:B:536:SER:O	2.49	0.42
1:C:384:SER:HB3	1:C:396:MET:HB2	2.00	0.42
1:A:497:THR:OG1	1:A:499:SER:OG	2.24	0.42
1:B:282:VAL:CG2	1:B:565:LEU:HG	2.50	0.42
1:B:469:ALA:HB1	1:B:517:VAL:HG23	2.01	0.42
1:A:303:ASP:OD1	1:A:303:ASP:C	2.58	0.42
1:A:380:MET:HG2	6:A:714:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:ILE:O	1:C:398:ARG:HA	2.20	0.42
1:D:470:LEU:HD12	1:D:474:HIS:O	2.20	0.42
1:B:510:ARG:NH2	1:B:538:GLU:HG2	2.35	0.41
1:D:416:ARG:NH2	1:D:444:GLU:HG3	2.34	0.41
1:B:467:GLY:HA3	1:B:515:ALA:HB2	2.02	0.41
1:D:317:ARG:HA	6:D:728:HOH:O	2.20	0.41
1:B:540:TYR:HB2	1:B:547:TRP:CH2	2.56	0.41
1:D:434:TYR:CD1	2:H:658:PRO:HG2	2.56	0.41
1:A:377:LEU:HD12	1:A:378:GLY:N	2.36	0.41
1:C:534:LEU:O	1:C:556:GLN:HA	2.21	0.41
1:C:284:LEU:HD11	1:C:312:LEU:HD22	2.03	0.41
1:B:281:GLU:HB2	1:B:518:LEU:HG	2.03	0.41
1:C:283:LEU:HD22	1:C:516:THR:CG2	2.51	0.41
1:D:393:HIS:NE2	6:D:704:HOH:O	2.36	0.41
1:D:510:ARG:HH21	1:D:538:GLU:HG2	1.84	0.41
1:A:284:LEU:HD12	1:A:300:GLU:O	2.20	0.41
1:A:315:ILE:HB	1:A:347:GLU:OE1	2.21	0.41
1:B:461:THR:O	1:B:463:ARG:HG3	2.22	0.40
1:A:369:ARG:HB3	1:A:372:ALA:HB2	2.04	0.40
1:A:493:TYR:OH	1:A:498:ASP:HA	2.22	0.40
1:B:301:LYS:HE2	1:B:310:SER:OG	2.22	0.40
1:C:409:LEU:HB3	6:C:771:HOH:O	2.21	0.40
1:C:507:THR:HG23	1:C:538:GLU:OE1	2.21	0.40
1:B:545:ASP:O	1:B:545:ASP:CG	2.60	0.40
1:D:409:LEU:HB3	1:D:410:GLY:H	1.69	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:765:HOH:O	6:B:848:HOH:O[2_646]	1.86	0.34
6:A:836:HOH:O	6:A:839:HOH:O[2_555]	2.01	0.19
6:B:867:HOH:O	6:D:817:HOH:O[2_656]	2.01	0.19
6:A:751:HOH:O	6:A:763:HOH:O[2_545]	2.07	0.13
1:A:291:SER:CB	6:A:810:HOH:O[2_555]	2.10	0.10
6:C:796:HOH:O	6:C:874:HOH:O[2_645]	2.10	0.10
6:A:781:HOH:O	6:C:873:HOH:O[2_655]	2.16	0.04

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	281/301 (93%)	273 (97%)	8 (3%)	0	100	100
1	B	282/301 (94%)	267 (95%)	15 (5%)	0	100	100
1	C	282/301 (94%)	272 (96%)	10 (4%)	0	100	100
1	D	283/301 (94%)	269 (95%)	14 (5%)	0	100	100
2	E	6/15 (40%)	6 (100%)	0	0	100	100
2	F	5/15 (33%)	5 (100%)	0	0	100	100
2	G	6/15 (40%)	6 (100%)	0	0	100	100
2	H	6/15 (40%)	6 (100%)	0	0	100	100
All	All	1151/1264 (91%)	1104 (96%)	47 (4%)	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	226/248 (91%)	225 (100%)	1 (0%)	91	96
1	B	227/248 (92%)	221 (97%)	6 (3%)	46	64
1	C	227/248 (92%)	226 (100%)	1 (0%)	91	96
1	D	221/248 (89%)	220 (100%)	1 (0%)	88	95
2	E	5/10 (50%)	5 (100%)	0	100	100
2	F	3/10 (30%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	5/10 (50%)	5 (100%)	0	100	100
2	H	4/10 (40%)	4 (100%)	0	100	100
All	All	918/1032 (89%)	909 (99%)	9 (1%)	76	87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	317	ARG
1	B	305	LYS
1	B	338	ASP
1	B	361	SER
1	B	390	SER
1	B	546	SER
1	B	559	ASP
1	C	546	SER
1	D	392	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	413	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

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	EDO	A	602	-	3,3,3	0.53	0	2,2,2	0.10	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	EDO	A	602	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	285/301 (94%)	0.44	10 (3%)	44	47	11, 20, 34, 68	0
1	B	285/301 (94%)	0.69	13 (4%)	32	35	20, 27, 44, 86	0
1	C	284/301 (94%)	0.37	7 (2%)	57	59	7, 16, 30, 62	0
1	D	286/301 (95%)	0.87	22 (7%)	13	14	27, 34, 47, 77	0
2	E	8/15 (53%)	2.82	4 (50%)	0	0	26, 28, 36, 44	0
2	F	7/15 (46%)	1.35	2 (28%)	0	0	28, 35, 51, 52	0
2	G	8/15 (53%)	2.11	4 (50%)	0	0	27, 29, 38, 42	0
2	H	8/15 (53%)	2.28	4 (50%)	0	0	30, 45, 56, 63	0
All	All	1171/1264 (92%)	0.63	66 (5%)	24	27	7, 25, 44, 86	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	567	GLU	8.3
1	D	279	ALA	8.1
1	B	279	ALA	6.8
2	E	662	PRO	6.7
1	D	352	THR	6.4
1	B	352	THR	6.3
1	A	279	ALA	5.8
1	C	351	TYR	5.8
1	C	279	ALA	5.6
1	B	329	ASP	5.3
2	E	656	GLY	5.2
1	A	351	TYR	4.8
1	D	567	GLU	4.8
2	H	656	GLY	4.8
1	A	352	THR	4.7
2	E	663	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	353	ALA	4.6
1	B	328	HIS	4.3
1	D	280	ASN	3.8
2	G	663	VAL	3.7
2	F	655	GLY	3.4
1	A	280	ASN	3.3
2	G	662	PRO	3.3
2	G	660	GLY	3.1
1	C	280	ASN	3.1
1	B	566	ARG	3.0
1	D	329	ASP	2.9
1	B	351	TYR	2.9
1	D	351	TYR	2.9
2	H	663	VAL	2.9
1	B	402	ASN	2.9
2	H	662	PRO	2.8
1	A	567	GLU	2.8
1	C	566	ARG	2.7
1	C	329	ASP	2.6
1	D	340	ARG	2.6
2	G	657	PRO	2.6
1	D	344	SER	2.5
1	B	390	SER	2.5
1	D	546	SER	2.5
1	B	280	ASN	2.4
1	D	497	THR	2.4
1	B	358	VAL	2.4
1	C	357	GLY	2.4
1	D	536	SER	2.3
1	B	547	TRP	2.3
1	A	437	LEU	2.3
1	A	350	ASP	2.3
1	D	410	GLY	2.3
1	C	328	HIS	2.3
1	D	333	VAL	2.3
2	E	658	PRO	2.3
1	D	326	SER	2.2
1	D	346	VAL	2.2
2	F	656	GLY	2.2
1	D	412	MET	2.1
1	D	360	TYR	2.1
1	B	298	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	329	ASP	2.1
1	D	537	ILE	2.1
1	A	516	THR	2.1
1	A	546	SER	2.1
1	D	357	GLY	2.1
1	D	380	MET	2.0
1	D	299	VAL	2.0
2	H	660	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, 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(Å^2)	Q<0.9
3	NA	A	601	1/1	0.78	0.16	30,30,30,30	0
4	EDO	A	602	4/4	0.80	0.33	20,20,20,20	0
3	NA	C	601	1/1	0.81	0.19	30,30,30,30	0
3	NA	B	601	1/1	0.89	0.25	39,39,39,39	0
3	NA	B	602	1/1	0.92	0.12	36,36,36,36	0
5	CL	D	601	1/1	0.93	0.18	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.