



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:45 PM UTC

PDB ID : 6TTK / pdb_00006ttk
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 ⓘ 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:

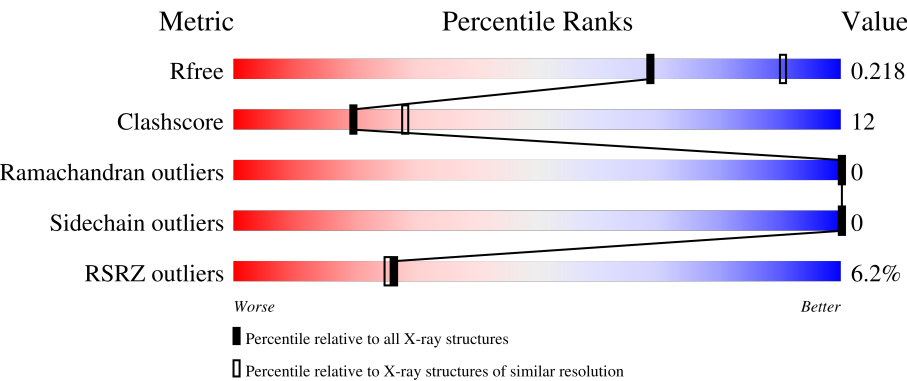
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (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 $\leq 5\%$. 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	301	4% 72% 21% • 5%
1	B	301	4% 66% 27% • 5%
1	C	301	2% 71% 21% • 6%
1	D	301	10% 75% 18% • 5%

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Mol	Chain	Length	Quality of chain
2	E	15	20%27%20%7%47%
2	F	15	13%27%13%7%53%
2	G	15	13%53%47%
2	H	15	33%33%13%7%47%

2 Entry composition

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

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

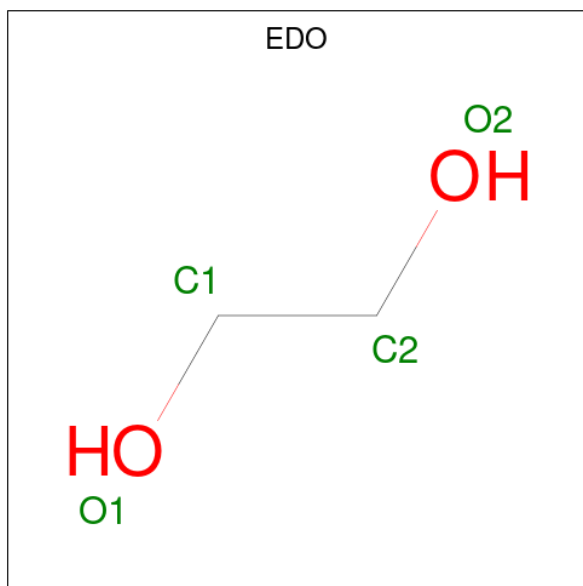
- Molecule 2 is a protein called DVL1.

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

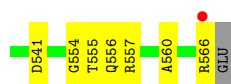
- Molecule 6 is water.

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

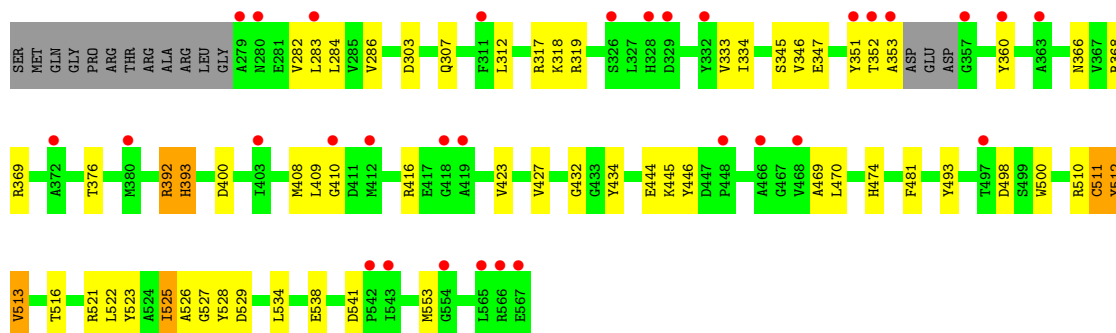
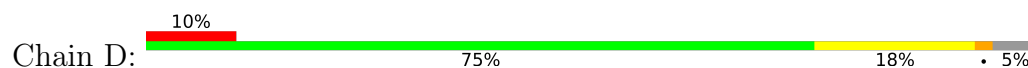
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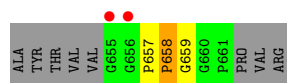
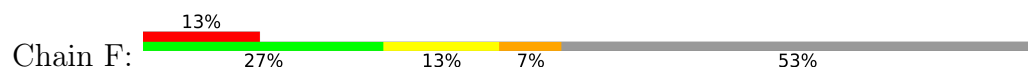
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	188	Total 188	O 188	0	0
6	D	122	Total 122	O 122	0	0
6	F	2	Total 2	O 2	0	0
6	H	1	Total 1	O 1	0	0
6	E	2	Total 2	O 2	0	0



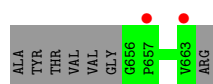
• Molecule 1: Kelch-like protein 12



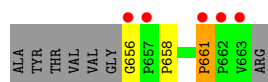
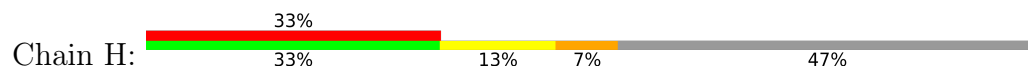
• Molecule 2: DVL1



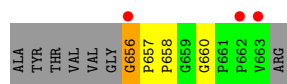
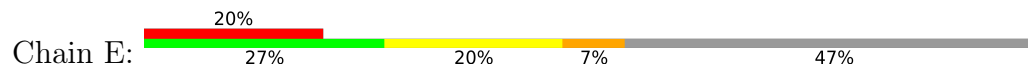
• Molecule 2: DVL1



• Molecule 2: DVL1



• Molecule 2: DVL1



4 Data and refinement statistics

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) 99.5 (79.98-2.38)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	2442 reflections (5.17%)	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)	0.36 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

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: EDO, CL, NA

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	0.89	13/2189 (0.6%)	0.85	3/2982 (0.1%)
1	B	0.89	10/2191 (0.5%)	0.90	14/2984 (0.5%)
1	C	0.91	17/2192 (0.8%)	0.88	8/2987 (0.3%)
1	D	0.80	10/2172 (0.5%)	0.87	10/2962 (0.3%)
2	E	2.62	1/50 (2.0%)	2.99	7/70 (10.0%)
2	F	2.52	1/39 (2.6%)	2.74	4/53 (7.5%)
2	G	0.26	0/50	0.36	0/70
2	H	2.27	1/48 (2.1%)	2.20	2/67 (3.0%)
All	All	0.92	53/8931 (0.6%)	0.93	48/12175 (0.4%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	657	PRO	CA-C	-9.99	1.45	1.52
1	A	282	VAL	C-O	-8.42	1.13	1.23
1	C	396	MET	C-O	-8.15	1.13	1.23
2	F	657	PRO	N-CD	-7.54	1.37	1.47
1	C	456	VAL	C-O	-7.40	1.16	1.24
1	C	380	MET	C-O	-7.38	1.14	1.23
2	H	661	PRO	C-O	-7.22	1.18	1.24
1	C	443	VAL	C-O	-6.93	1.17	1.24
1	C	444	GLU	C-O	-6.87	1.15	1.23
1	C	409	LEU	C-O	-6.83	1.15	1.24
1	C	398	ARG	C-O	-6.82	1.15	1.24
1	D	511[A]	CYS	CA-C	6.76	1.60	1.52
1	D	511[B]	CYS	CA-C	6.76	1.60	1.52
1	D	512	TYR	C-O	-6.59	1.15	1.23
1	C	427	VAL	C-O	-6.53	1.17	1.24
1	A	496	ARG	C-O	-6.51	1.15	1.24
1	B	547	TRP	C-O	-6.50	1.16	1.24
1	A	318	LYS	C-O	-6.17	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	ARG	C-O	-6.16	1.16	1.23
1	B	545	ASP	C-O	-6.15	1.15	1.23
1	B	453	TRP	C-O	-6.13	1.16	1.24
1	A	551	THR	C-O	-6.01	1.16	1.23
1	C	426	GLY	C-O	-5.94	1.15	1.23
1	C	455	ASN	C-O	-5.94	1.16	1.23
1	A	316	THR	C-O	-5.83	1.17	1.24
1	A	531	ASN	C-O	-5.82	1.16	1.24
1	B	297	ASP	C-O	-5.78	1.16	1.24
1	A	530	GLY	C-O	-5.72	1.16	1.24
1	C	397	GLU	C-O	-5.71	1.16	1.23
1	D	526	ALA	C-O	-5.69	1.19	1.24
1	C	526	ALA	C-O	-5.68	1.18	1.24
1	A	459	MET	C-O	-5.66	1.16	1.23
1	C	408	MET	C-O	-5.66	1.17	1.23
1	B	456	VAL	N-CA	-5.63	1.39	1.46
1	A	458	PRO	C-O	-5.60	1.17	1.23
1	A	460	ALA	C-O	-5.60	1.17	1.24
1	D	307	GLN	N-CA	-5.57	1.38	1.46
1	C	527	GLY	C-O	-5.56	1.16	1.24
1	B	546	SER	C-O	-5.45	1.17	1.23
1	A	528	TYR	C-O	-5.36	1.18	1.24
1	D	369	ARG	C-O	-5.26	1.18	1.24
1	C	428	ILE	C-O	-5.23	1.18	1.24
1	D	527	GLY	C-O	-5.20	1.17	1.23
1	C	397	GLU	CD-OE1	-5.16	1.15	1.25
1	D	432	GLY	C-O	-5.16	1.16	1.24
1	B	309	TRP	C-O	-5.15	1.17	1.23
1	A	519	ARG	C-O	-5.14	1.17	1.23
1	D	392	ARG	C-O	-5.08	1.17	1.23
1	B	454	THR	C-O	-5.07	1.17	1.23
1	B	450	THR	C-O	-5.07	1.17	1.24
1	A	317	ARG	CA-C	-5.07	1.46	1.52
1	D	513	VAL	C-O	-5.05	1.18	1.24
1	B	346	VAL	C-O	-5.04	1.18	1.24

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	MET	N-CA-C	14.94	131.30	112.92
2	F	659	GLY	N-CA-C	-9.87	95.05	112.22
2	E	657	PRO	O-C-N	9.73	125.73	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	525	ILE	N-CA-C	8.56	120.22	107.80
1	D	393	HIS	N-CA-C	8.52	123.49	109.95
1	B	369	ARG	N-CA-C	8.40	122.12	108.34
1	D	511[A]	CYS	N-CA-C	8.07	122.58	109.59
1	D	511[B]	CYS	N-CA-C	8.07	122.58	109.59
1	D	369	ARG	N-CA-C	7.61	121.61	108.76
1	C	428	ILE	N-CA-C	7.40	118.53	108.17
1	D	525	ILE	N-CA-C	7.40	118.53	107.80
1	C	343	LEU	N-CA-C	7.27	121.50	109.95
1	D	432	GLY	N-CA-C	7.14	124.80	111.80
1	C	410	GLY	N-CA-C	7.02	120.00	111.93
2	E	656	GLY	CA-C-N	-6.94	114.66	119.66
2	E	656	GLY	C-N-CA	-6.94	114.66	119.66
1	D	511[A]	CYS	CA-C-O	-6.85	113.37	121.11
1	D	511[B]	CYS	CA-C-O	-6.85	113.37	121.11
1	B	345	SER	N-CA-C	6.82	120.57	110.48
1	C	455	ASN	CA-C-N	6.70	133.93	122.67
1	C	455	ASN	C-N-CA	6.70	133.93	122.67
2	E	657	PRO	CA-C-N	-5.91	113.67	119.76
2	E	657	PRO	C-N-CA	-5.91	113.67	119.76
1	B	296	ILE	N-CA-C	5.88	117.39	108.80
1	B	546	SER	N-CA-C	5.88	116.85	108.74
1	B	348	CYS	N-CA-C	5.77	118.62	109.50
1	B	455	ASN	N-CA-C	5.76	119.00	110.48
2	E	660	GLY	CA-C-N	-5.60	114.61	120.38
2	E	660	GLY	C-N-CA	-5.60	114.61	120.38
1	D	360	TYR	CA-C-N	5.54	128.74	120.87
1	D	360	TYR	C-N-CA	5.54	128.74	120.87
1	B	544	ILE	CA-C-N	5.52	129.96	122.07
1	B	544	ILE	C-N-CA	5.52	129.96	122.07
2	F	657	PRO	CA-C-N	-5.46	113.93	119.83
2	F	657	PRO	C-N-CA	-5.46	113.93	119.83
1	A	495	ILE	N-CA-C	5.44	116.17	110.62
1	B	456	VAL	N-CA-C	-5.40	100.04	108.95
1	B	457	THR	CA-C-N	-5.24	114.84	120.03
1	B	457	THR	C-N-CA	-5.24	114.84	120.03
1	B	547	TRP	N-CA-C	5.21	117.01	108.52
2	H	656	GLY	CA-C-N	-5.19	115.03	120.38
2	H	656	GLY	C-N-CA	-5.19	115.03	120.38
2	F	658	PRO	N-CA-C	5.16	118.97	111.03
1	C	357	GLY	CA-C-N	-5.12	115.83	122.94
1	C	357	GLY	C-N-CA	-5.12	115.83	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	305	LYS	CA-C-N	5.09	128.06	120.31
1	B	305	LYS	C-N-CA	5.09	128.06	120.31
1	A	280	ASN	N-CA-C	5.07	116.97	107.99

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	2143	0	2044	44	1
1	B	2142	0	2038	71	0
1	C	2143	0	2033	38	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	16	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	196	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 12.

All (196) 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:D:351:TYR:C	1:D:353:ALA:N	2.48	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
1:B:535:SER:HB2	1:B:554:GLY:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:351:TYR:C	1:D:353:ALA:H	2.05	0.63
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: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:B:498:ASP:CG	1:B:498:ASP:O	2.44	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: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:B:462:LYS:NZ	6:B:717:HOH:O	2.31	0.58
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:D:351:TYR:O	1:D:352:THR:C	2.47	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: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:C:300:GLU:CD	1:C:555[A]:THR:HG23	2.35	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:A:365:MET:HE1	1:A:369:ARG:HB2	1.93	0.49
1:C:369:ARG:HH21	1:C:397:GLU:HG2	1.77	0.49
1:A:332:TYR:OH	6:A:702:HOH:O	2.15	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:395:SER:HB2	1:B:408:MET:HE1	1.94	0.48
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:LEU:HD12	1:D:409:LEU:N	2.30	0.46
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:303:ASP:OD1	1:A:303:ASP:C	2.58	0.45
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:B:545:ASP:O	1:B:545:ASP:CG	2.60	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:C:521:ARG:HD3	1:C:541:ASP:CG	2.43	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:B:281:GLU:C	1:B:518:LEU:HD11	2.44	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:506:MET:HE1	1:B:510:ARG:HB2	2.02	0.42
1:B:510:ARG:NH1	1:B:536:SER:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:380:MET:HG2	6:A:714:HOH:O	2.19	0.42
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:415:ALA:C	1:B:416:ARG:HG3	2.43	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:B:565:LEU:HD12	1:B:565:LEU:C	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	226 (100%)	0	100	100
1	B	227/248 (92%)	227 (100%)	0	100	100
1	C	227/248 (92%)	227 (100%)	0	100	100
1	D	221/248 (89%)	221 (100%)	0	100	100
2	E	5/10 (50%)	5 (100%)	0	100	100
2	F	3/10 (30%)	3 (100%)	0	100	100
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%)	918 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	452	HIS
1	D	452	HIS
1	D	474	HIS
1	D	486	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 oligosaccharides 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

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	285/301 (94%)	0.35	11 (3%) 43 43	11, 20, 34, 68	0
1	B	285/301 (94%)	0.71	13 (4%) 37 37	15, 27, 44, 86	1 (0%)
1	C	284/301 (94%)	0.17	6 (2%) 63 62	7, 15, 30, 62	2 (0%)
1	D	286/301 (95%)	1.14	31 (10%) 11 9	20, 34, 47, 77	1 (0%)
2	E	8/15 (53%)	1.61	3 (37%) 1 0	26, 28, 36, 44	0
2	F	7/15 (46%)	1.60	2 (28%) 1 1	28, 35, 51, 52	0
2	G	8/15 (53%)	1.53	2 (25%) 2 1	27, 29, 38, 42	0
2	H	8/15 (53%)	2.34	5 (62%) 0 0	30, 45, 56, 63	0
All	All	1171/1264 (92%)	0.63	73 (6%) 26 25	7, 25, 44, 86	4 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	ALA	5.2
1	D	279	ALA	5.1
1	B	352	THR	4.9
1	A	352	THR	4.7
1	D	352	THR	4.5
1	C	279	ALA	4.3
1	A	357	GLY	4.3
1	D	567	GLU	4.1
1	A	279	ALA	4.1
1	D	357	GLY	4.1
2	H	656	GLY	3.9
1	A	358	VAL	3.8
1	D	353	ALA	3.7
1	D	497	THR	3.7
1	D	351	TYR	3.6
1	B	328	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	329	ASP	3.4
1	B	567	GLU	3.4
1	C	351	TYR	3.3
1	B	351	TYR	3.3
1	C	352	THR	3.2
1	A	566	ARG	3.1
1	D	418	GLY	3.1
1	D	311	PHE	3.1
1	D	280	ASN	3.1
2	E	662	PRO	3.0
1	B	565	LEU	2.9
1	D	412	MET	2.9
1	A	280	ASN	2.9
2	F	655	GLY	2.8
2	H	663	VAL	2.8
1	D	403	ILE	2.8
2	F	656	GLY	2.7
1	A	351	TYR	2.6
1	D	360	TYR	2.6
2	H	662	PRO	2.6
1	A	281	GLU	2.6
1	D	566	ARG	2.6
1	D	380	MET	2.6
1	B	357	GLY	2.6
1	D	363	ALA	2.5
1	A	329	ASP	2.5
2	E	656	GLY	2.5
1	D	332	TYR	2.4
2	E	663	VAL	2.4
1	C	357	GLY	2.4
1	D	326	SER	2.4
2	G	663	VAL	2.4
1	A	567	GLU	2.4
1	D	542	PRO	2.4
1	D	468	VAL	2.4
2	H	657	PRO	2.3
1	B	368	ARG	2.3
1	C	328	HIS	2.3
1	D	328	HIS	2.3
2	H	661	PRO	2.3
1	D	466	ALA	2.3
1	D	410	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	290	GLY	2.2
1	D	372	ALA	2.2
1	D	543	ILE	2.2
1	B	390	SER	2.2
1	D	283	LEU	2.1
1	A	328	HIS	2.1
1	D	554	GLY	2.1
1	C	566	ARG	2.1
1	B	306	THR	2.1
1	D	329	ASP	2.1
2	G	657	PRO	2.1
1	B	472	ASN	2.0
1	D	419	ALA	2.0
1	D	565	LEU	2.0
1	D	448	PRO	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	NA	A	601	1/1	0.76	0.11	30,30,30,30	0
4	EDO	A	602	4/4	0.77	0.21	20,20,20,20	0
3	NA	C	601	1/1	0.82	0.10	30,30,30,30	0
3	NA	B	601	1/1	0.86	0.16	39,39,39,39	0
5	CL	D	601	1/1	0.94	0.16	30,30,30,30	0
3	NA	B	602	1/1	0.95	0.06	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.