



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:42 AM GMT

PDB ID : 2Y0N
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN DOSAGE COMPENSATION FACTORS MSL1 AND MSL3
Authors : Kadlec, J.; Hallacli, E.; Lipp, M.; Holz, H.; Sanchez Weatherby, J.; Cusack, S.; Akhtar, A.
Deposited on : 2010-12-04
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

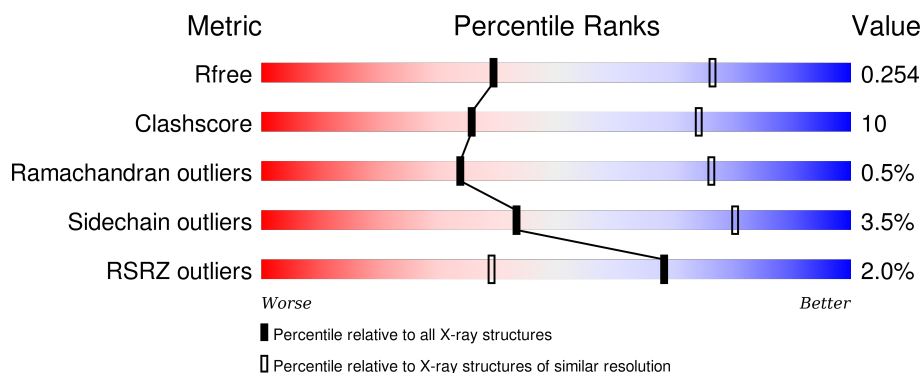
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	211	<div> <div> <div>2%</div> <div>62%</div> <div>14%</div> <div>•</div> <div>22%</div> </div> </div>
1	B	211	<div> <div> <div>2%</div> <div>61%</div> <div>15%</div> <div>•</div> <div>22%</div> </div> </div>
1	C	211	<div> <div> <div>2%</div> <div>63%</div> <div>12%</div> <div>•</div> <div>22%</div> </div> </div>
1	D	211	<div> <div> <div>3%</div> <div>63%</div> <div>13%</div> <div>•</div> <div>22%</div> </div> </div>
2	E	56	<div> <div> <div>2%</div> <div>52%</div> <div>18%</div> <div>30%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	56	 54% 11% 36%
2	G	56	 2% 34% 18% 48%
2	H	56	 30% 21% 48%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6492 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 MALE-SPECIFIC LETHAL 3 HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1359	894	216	244	5			
1	B	165	Total	C	N	O	S	0	0	0
			1359	894	216	244	5			
1	C	164	Total	C	N	O	S	0	0	0
			1355	893	215	242	5			
1	D	164	Total	C	N	O	S	0	0	0
			1355	893	215	242	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	MET	-	EXPRESSION TAG	UNP Q8N5Y2
A	166	GLY	-	EXPRESSION TAG	UNP Q8N5Y2
A	290	TYR	-	INSERTION	UNP Q8N5Y2
A	291	ASP	-	INSERTION	UNP Q8N5Y2
A	292	ILE	-	INSERTION	UNP Q8N5Y2
A	293	PRO	-	INSERTION	UNP Q8N5Y2
A	294	PRO	-	INSERTION	UNP Q8N5Y2
A	295	THR	-	INSERTION	UNP Q8N5Y2
A	296	THR	-	INSERTION	UNP Q8N5Y2
A	440	GLU	-	INSERTION	UNP Q8N5Y2
A	441	PHE	-	INSERTION	UNP Q8N5Y2
B	165	MET	-	EXPRESSION TAG	UNP Q8N5Y2
B	166	GLY	-	EXPRESSION TAG	UNP Q8N5Y2
B	290	TYR	-	INSERTION	UNP Q8N5Y2
B	291	ASP	-	INSERTION	UNP Q8N5Y2
B	292	ILE	-	INSERTION	UNP Q8N5Y2
B	293	PRO	-	INSERTION	UNP Q8N5Y2
B	294	PRO	-	INSERTION	UNP Q8N5Y2
B	295	THR	-	INSERTION	UNP Q8N5Y2
B	296	THR	-	INSERTION	UNP Q8N5Y2
B	440	GLU	-	INSERTION	UNP Q8N5Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	441	PHE	-	INSERTION	UNP Q8N5Y2
C	165	MET	-	EXPRESSION TAG	UNP Q8N5Y2
C	166	GLY	-	EXPRESSION TAG	UNP Q8N5Y2
C	290	TYR	-	INSERTION	UNP Q8N5Y2
C	291	ASP	-	INSERTION	UNP Q8N5Y2
C	292	ILE	-	INSERTION	UNP Q8N5Y2
C	293	PRO	-	INSERTION	UNP Q8N5Y2
C	294	PRO	-	INSERTION	UNP Q8N5Y2
C	295	THR	-	INSERTION	UNP Q8N5Y2
C	296	THR	-	INSERTION	UNP Q8N5Y2
C	440	GLU	-	INSERTION	UNP Q8N5Y2
C	441	PHE	-	INSERTION	UNP Q8N5Y2
D	165	MET	-	EXPRESSION TAG	UNP Q8N5Y2
D	166	GLY	-	EXPRESSION TAG	UNP Q8N5Y2
D	290	TYR	-	INSERTION	UNP Q8N5Y2
D	291	ASP	-	INSERTION	UNP Q8N5Y2
D	292	ILE	-	INSERTION	UNP Q8N5Y2
D	293	PRO	-	INSERTION	UNP Q8N5Y2
D	294	PRO	-	INSERTION	UNP Q8N5Y2
D	295	THR	-	INSERTION	UNP Q8N5Y2
D	296	THR	-	INSERTION	UNP Q8N5Y2
D	440	GLU	-	INSERTION	UNP Q8N5Y2
D	441	PHE	-	INSERTION	UNP Q8N5Y2

- Molecule 2 is a protein called MALE-SPECIFIC LETHAL 1 HOMOLOG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	39	Total	C	N	O	0	0	0
			314	217	46	51			
2	F	36	Total	C	N	O	0	0	0
			290	201	43	46			
2	G	29	Total	C	N	O	0	0	0
			230	159	35	36			
2	H	29	Total	C	N	O	0	0	0
			230	159	35	36			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	542	GLY	-	EXPRESSION TAG	UNP Q6PDM1
E	543	ALA	-	EXPRESSION TAG	UNP Q6PDM1
E	544	MET	-	EXPRESSION TAG	UNP Q6PDM1

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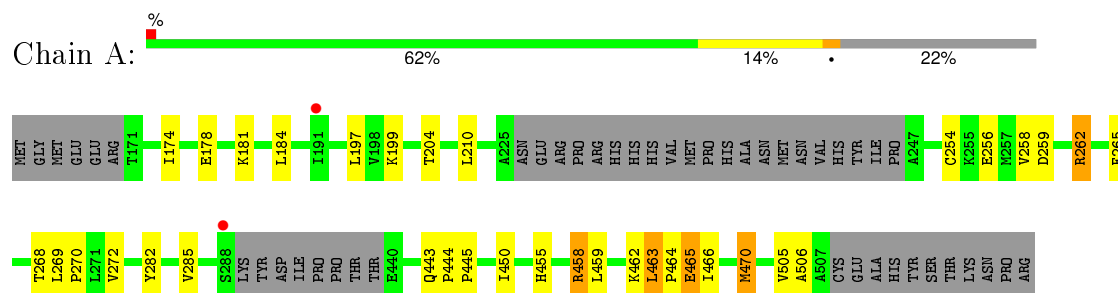
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Chain	Residue	Modelled	Actual	Comment	Reference
F	542	GLY	-	EXPRESSION TAG	UNP Q6PDM1
F	543	ALA	-	EXPRESSION TAG	UNP Q6PDM1
F	544	MET	-	EXPRESSION TAG	UNP Q6PDM1
G	542	GLY	-	EXPRESSION TAG	UNP Q6PDM1
G	543	ALA	-	EXPRESSION TAG	UNP Q6PDM1
G	544	MET	-	EXPRESSION TAG	UNP Q6PDM1
H	542	GLY	-	EXPRESSION TAG	UNP Q6PDM1
H	543	ALA	-	EXPRESSION TAG	UNP Q6PDM1
H	544	MET	-	EXPRESSION TAG	UNP Q6PDM1

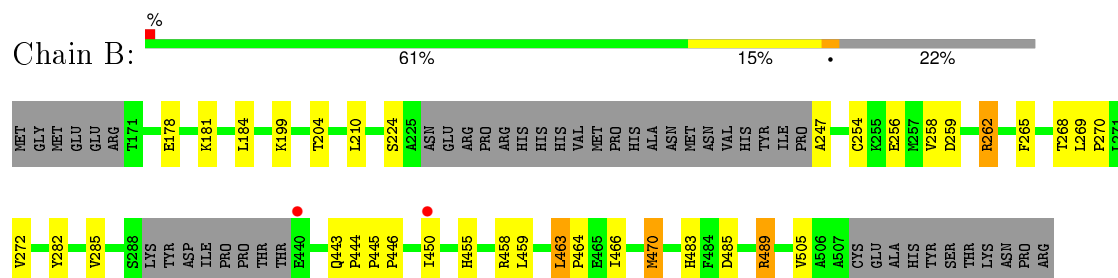
3 Residue-property plots [i](#)

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

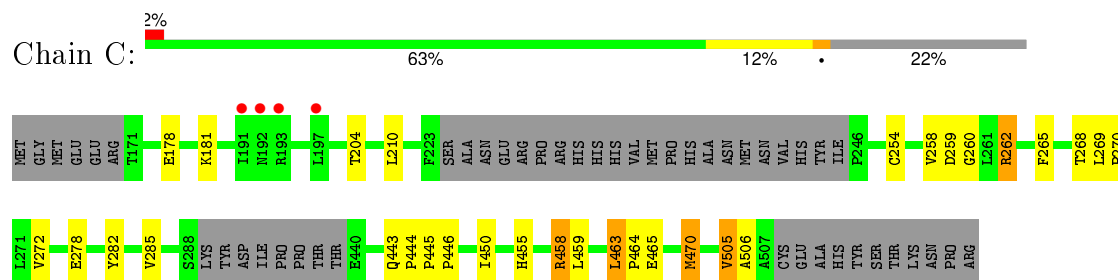
• Molecule 1: MALE-SPECIFIC LETHAL 3 HOMOLOG



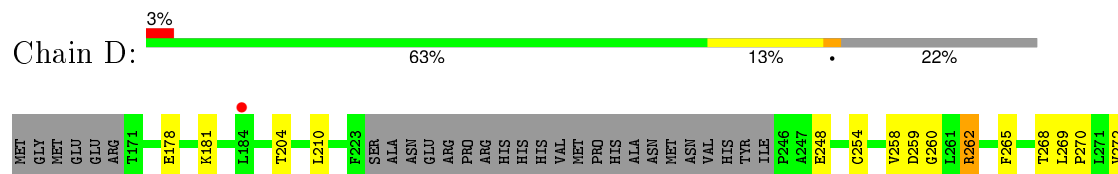
• Molecule 1: MALE-SPECIFIC LETHAL 3 HOMOLOG

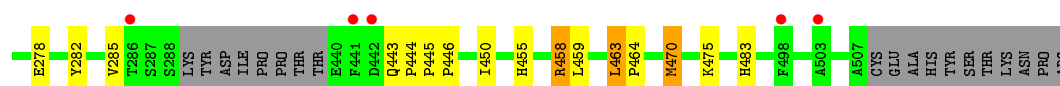


• Molecule 1: MALE-SPECIFIC LETHAL 3 HOMOLOG

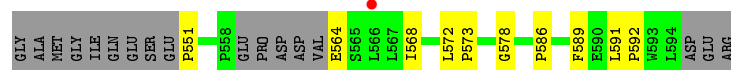


• Molecule 1: MALE-SPECIFIC LETHAL 3 HOMOLOG

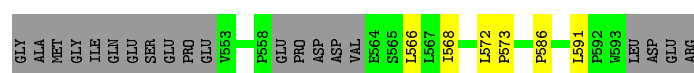




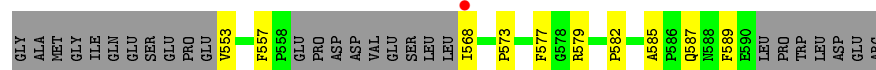
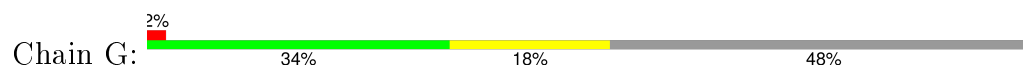
● Molecule 2: MALE-SPECIFIC LETHAL 1 HOMOLOG



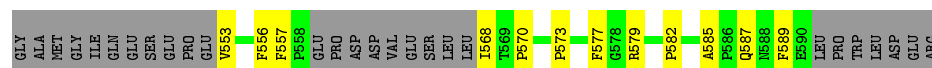
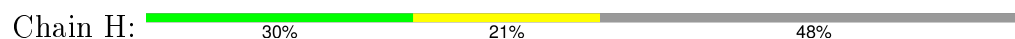
● Molecule 2: MALE-SPECIFIC LETHAL 1 HOMOLOG



● Molecule 2: MALE-SPECIFIC LETHAL 1 HOMOLOG



● Molecule 2: MALE-SPECIFIC LETHAL 1 HOMOLOG



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.23Å 127.27Å 79.68Å 90.00° 118.46° 90.00°	Depositor
Resolution (Å)	46.13 – 3.00 38.11 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.6 (46.13-3.00) 93.6 (38.11-3.00)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0085	Depositor
R, R_{free}	0.232 , 0.253 0.232 , 0.254	Depositor DCC
R_{free} test set	1260 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	99.4	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.3	EDS
Estimated twinning fraction	0.468 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25053 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6492	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.45	0/1392	0.55	0/1883
1	B	0.44	0/1392	0.55	0/1883
1	C	0.49	1/1389 (0.1%)	0.54	0/1879
1	D	0.45	0/1389	0.54	0/1879
2	E	0.51	0/327	0.61	0/449
2	F	0.53	0/302	0.61	0/415
2	G	0.54	0/239	0.61	0/327
2	H	0.54	0/239	0.61	0/327
All	All	0.47	1/6669 (0.0%)	0.56	0/9042

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	505	VAL	CB-CG1	-7.78	1.36	1.52

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	1359	0	1374	30	0
1	B	1359	0	1374	29	0
1	C	1355	0	1372	26	0
1	D	1355	0	1372	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	314	0	320	10	0
2	F	290	0	295	5	0
2	G	230	0	234	11	0
2	H	230	0	234	12	0
All	All	6492	0	6575	127	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 10.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:LYS:NZ	2:E:551:PRO:HB3	1.92	0.84
1:A:268:THR:HG22	1:A:272:VAL:HG12	1.69	0.74
1:D:475:LYS:HZ1	2:E:551:PRO:HB3	1.54	0.73
1:D:248:GLU:HG3	1:D:483:HIS:CE1	2.23	0.72
1:D:268:THR:HG22	1:D:272:VAL:HG12	1.73	0.70
1:C:259:ASP:OD1	1:C:262:ARG:NH1	2.25	0.69
1:B:268:THR:CG2	1:B:272:VAL:HG12	2.23	0.69
1:A:268:THR:CG2	1:A:272:VAL:HG12	2.22	0.69
1:C:443:GLN:HB3	1:C:444:PRO:HD2	1.75	0.68
1:B:268:THR:HG22	1:B:272:VAL:HG12	1.76	0.68
1:D:210:LEU:HB3	1:D:258:VAL:CG1	2.24	0.68
1:D:259:ASP:OD1	1:D:262:ARG:NH1	2.26	0.67
1:B:259:ASP:OD1	1:B:262:ARG:NH1	2.27	0.67
1:D:443:GLN:HB3	1:D:444:PRO:HD2	1.76	0.67
1:A:210:LEU:HB3	1:A:258:VAL:CG1	2.24	0.66
1:C:268:THR:HG22	1:C:272:VAL:HG12	1.78	0.66
1:C:210:LEU:HB3	1:C:258:VAL:CG1	2.27	0.65
1:B:210:LEU:HB3	1:B:258:VAL:CG1	2.25	0.65
1:B:443:GLN:HB3	1:B:444:PRO:HD2	1.78	0.65
1:A:259:ASP:OD1	1:A:262:ARG:NH1	2.30	0.64
1:A:443:GLN:HB3	1:A:444:PRO:HD2	1.80	0.64
1:C:443:GLN:HB3	1:C:444:PRO:CD	2.28	0.63
1:D:268:THR:CG2	1:D:272:VAL:HG12	2.29	0.63
1:D:443:GLN:HB3	1:D:444:PRO:CD	2.28	0.63
1:C:470:MET:HG2	2:G:582:PRO:HD3	1.82	0.62
1:C:268:THR:CG2	1:C:272:VAL:HG12	2.30	0.62
1:A:443:GLN:HB3	1:A:444:PRO:CD	2.29	0.62
1:A:462:LYS:O	1:A:465:GLU:HG3	1.99	0.62
2:E:568:ILE:HD12	2:H:573:PRO:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:GLN:HB3	1:B:444:PRO:CD	2.30	0.61
2:F:568:ILE:HD12	2:G:573:PRO:HG3	1.82	0.61
1:B:247:ALA:O	1:B:483:HIS:CE1	2.55	0.59
1:B:247:ALA:O	1:B:483:HIS:HE1	1.85	0.59
1:A:455:HIS:HA	1:A:458:ARG:HG3	1.85	0.58
1:D:470:MET:HG2	2:H:582:PRO:HD3	1.86	0.58
1:D:475:LYS:HZ3	2:E:551:PRO:HB3	1.66	0.57
1:C:458:ARG:HD2	2:G:589:PHE:CE2	2.39	0.57
1:B:256:GLU:HG2	2:G:557:PHE:HE2	1.70	0.57
1:C:455:HIS:HA	1:C:458:ARG:HG3	1.86	0.57
1:C:505:VAL:HG12	1:C:506:ALA:N	2.20	0.57
1:D:455:HIS:HA	1:D:458:ARG:HG3	1.86	0.56
1:D:458:ARG:HD2	2:H:589:PHE:CE2	2.41	0.56
2:H:579:ARG:HH11	2:H:579:ARG:HG2	1.71	0.56
2:G:579:ARG:HH11	2:G:579:ARG:HG2	1.71	0.55
1:B:455:HIS:HA	1:B:458:ARG:HG3	1.88	0.55
1:A:256:GLU:HG2	2:H:557:PHE:HE2	1.72	0.55
2:G:568:ILE:HG23	2:H:585:ALA:HB2	1.88	0.55
1:A:270:PRO:HB3	1:A:282:TYR:CZ	2.42	0.55
1:B:459:LEU:HG	1:B:463:LEU:CD1	2.37	0.55
2:G:585:ALA:HB2	2:H:568:ILE:HG23	1.88	0.55
1:A:459:LEU:HG	1:A:463:LEU:CD1	2.38	0.54
1:D:270:PRO:HB3	1:D:282:TYR:CZ	2.43	0.54
1:B:270:PRO:HB3	1:B:282:TYR:CZ	2.43	0.54
1:C:285:VAL:HG11	1:C:450:ILE:HG21	1.89	0.54
1:A:459:LEU:HG	1:A:463:LEU:HD13	1.90	0.54
1:C:270:PRO:HB3	1:C:282:TYR:CZ	2.44	0.53
1:D:459:LEU:HG	1:D:463:LEU:CD1	2.39	0.52
1:D:285:VAL:HG11	1:D:450:ILE:HG21	1.91	0.52
1:B:210:LEU:HD22	1:B:258:VAL:HG13	1.92	0.52
2:F:572:LEU:HD12	2:F:573:PRO:HD2	1.92	0.52
1:A:285:VAL:HG11	1:A:450:ILE:HG21	1.91	0.51
1:B:459:LEU:HG	1:B:463:LEU:HD13	1.93	0.51
1:C:459:LEU:HG	1:C:463:LEU:CD1	2.40	0.51
1:B:285:VAL:HG11	1:B:450:ILE:HG21	1.92	0.50
1:D:459:LEU:HG	1:D:463:LEU:HD13	1.92	0.50
1:C:459:LEU:HG	1:C:463:LEU:HD13	1.93	0.50
1:B:463:LEU:N	1:B:464:PRO:HD2	2.27	0.50
1:A:268:THR:CG2	1:A:272:VAL:CG1	2.90	0.49
1:A:210:LEU:HD22	1:A:258:VAL:HG13	1.95	0.48
1:A:184:LEU:HB3	2:E:591:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LEU:N	1:A:464:PRO:HD2	2.29	0.48
1:C:265:PHE:CZ	1:C:269:LEU:HD13	2.49	0.48
1:D:210:LEU:HD22	1:D:258:VAL:HG13	1.96	0.47
1:C:210:LEU:HD22	1:C:258:VAL:HG13	1.97	0.47
1:D:265:PHE:CZ	1:D:269:LEU:HD13	2.50	0.47
1:B:184:LEU:HB3	2:F:591:LEU:HD21	1.97	0.47
1:B:485:ASP:O	1:B:489:ARG:HG2	2.15	0.47
1:B:268:THR:HG23	1:B:272:VAL:HG12	1.97	0.47
1:B:199:LYS:HB2	1:B:505:VAL:HG21	1.97	0.46
1:B:178:GLU:HA	1:B:181:LYS:HB2	1.97	0.46
1:C:178:GLU:HA	1:C:181:LYS:HB2	1.97	0.46
1:D:463:LEU:N	1:D:464:PRO:HD2	2.31	0.46
1:D:248:GLU:HG3	1:D:483:HIS:ND1	2.31	0.46
1:A:197:LEU:O	1:A:505:VAL:N	2.49	0.46
1:A:505:VAL:HG12	1:A:506:ALA:N	2.31	0.46
1:D:178:GLU:HA	1:D:181:LYS:HB2	1.98	0.46
1:C:272:VAL:HG23	2:G:587:GLN:HB3	1.98	0.45
1:C:463:LEU:N	1:C:464:PRO:HD2	2.31	0.45
1:A:265:PHE:CZ	1:A:269:LEU:HD13	2.52	0.45
1:A:178:GLU:HA	1:A:181:LYS:HB2	1.98	0.45
1:B:268:THR:CG2	1:B:272:VAL:CG1	2.92	0.45
1:C:505:VAL:HG12	1:C:506:ALA:H	1.80	0.45
1:D:445:PRO:HA	1:D:446:PRO:HD3	1.84	0.45
1:D:272:VAL:HG23	2:H:587:GLN:HB3	1.99	0.45
1:B:265:PHE:CZ	1:B:269:LEU:HD13	2.53	0.45
1:A:505:VAL:CG1	1:A:506:ALA:N	2.80	0.44
1:B:466:ILE:HG22	1:B:470:MET:CE	2.47	0.43
1:D:268:THR:CG2	1:D:272:VAL:CG1	2.95	0.43
1:B:285:VAL:CG1	1:B:450:ILE:HD13	2.49	0.43
2:E:572:LEU:HD12	2:E:573:PRO:HD2	2.00	0.43
1:C:445:PRO:HA	1:C:446:PRO:HD3	1.86	0.43
1:A:254:CYS:O	1:A:258:VAL:HG23	2.19	0.43
1:B:254:CYS:O	1:B:258:VAL:HG23	2.19	0.43
1:C:278:GLU:OE1	1:C:458:ARG:NH2	2.51	0.43
2:F:568:ILE:HD12	2:G:573:PRO:HB3	1.99	0.43
1:C:254:CYS:O	1:C:258:VAL:HG23	2.19	0.42
1:A:444:PRO:HA	1:A:445:PRO:HD2	1.94	0.42
1:A:285:VAL:CG1	1:A:450:ILE:HD13	2.50	0.42
1:B:199:LYS:HB2	1:B:505:VAL:CG2	2.49	0.42
1:A:466:ILE:HG22	1:A:470:MET:CE	2.49	0.42
1:C:268:THR:CG2	1:C:272:VAL:CG1	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:GLY:HA3	2:H:577:PHE:CE1	2.54	0.42
1:A:268:THR:HG22	1:A:272:VAL:CG1	2.46	0.41
1:A:458:ARG:HD2	2:E:589:PHE:CE2	2.55	0.41
1:B:444:PRO:HA	1:B:445:PRO:HD2	1.95	0.41
1:D:278:GLU:OE1	1:D:458:ARG:NH2	2.53	0.41
1:C:260:GLY:HA3	2:G:577:PHE:CE1	2.55	0.41
2:E:564:GLU:HG2	2:E:564:GLU:O	2.21	0.41
1:D:254:CYS:O	1:D:258:VAL:HG23	2.21	0.41
2:F:568:ILE:HD12	2:G:573:PRO:CG	2.51	0.41
2:H:579:ARG:HG2	2:H:579:ARG:NH1	2.34	0.41
1:A:199:LYS:HB2	1:A:505:VAL:HG21	2.02	0.41
2:E:578:GLY:HA3	2:H:556:PHE:O	2.21	0.41
1:A:174:ILE:HD12	1:A:464:PRO:HD3	2.02	0.40
1:B:445:PRO:HA	1:B:446:PRO:HD3	1.84	0.40
1:C:285:VAL:CG1	1:C:450:ILE:HD13	2.51	0.40
2:E:568:ILE:O	2:H:570:PRO:HA	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	159/211 (75%)	152 (96%)	7 (4%)	0	100	100
1	B	159/211 (75%)	152 (96%)	6 (4%)	1 (1%)	30	72
1	C	158/211 (75%)	151 (96%)	7 (4%)	0	100	100
1	D	158/211 (75%)	151 (96%)	7 (4%)	0	100	100
2	E	35/56 (62%)	30 (86%)	3 (9%)	2 (6%)	2	12
2	F	32/56 (57%)	30 (94%)	1 (3%)	1 (3%)	5	28
2	G	25/56 (45%)	23 (92%)	2 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	25/56 (45%)	23 (92%)	2 (8%)	0	100	100
All	All	751/1068 (70%)	712 (95%)	35 (5%)	4 (0%)	34	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	224	SER
2	E	586	PRO
2	F	586	PRO
2	E	592	PRO

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	150/193 (78%)	144 (96%)	6 (4%)	38	77
1	B	150/193 (78%)	145 (97%)	5 (3%)	45	82
1	C	150/193 (78%)	144 (96%)	6 (4%)	38	77
1	D	150/193 (78%)	145 (97%)	5 (3%)	45	82
2	E	36/50 (72%)	36 (100%)	0	100	100
2	F	33/50 (66%)	32 (97%)	1 (3%)	48	83
2	G	26/50 (52%)	25 (96%)	1 (4%)	40	78
2	H	26/50 (52%)	25 (96%)	1 (4%)	40	78
All	All	721/972 (74%)	696 (96%)	25 (4%)	43	80

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	THR
1	A	262	ARG
1	A	458	ARG
1	A	463	LEU

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Mol	Chain	Res	Type
1	A	465	GLU
1	A	470	MET
1	B	204	THR
1	B	262	ARG
1	B	463	LEU
1	B	470	MET
1	B	489	ARG
1	C	204	THR
1	C	262	ARG
1	C	458	ARG
1	C	463	LEU
1	C	465	GLU
1	C	470	MET
1	D	204	THR
1	D	262	ARG
1	D	458	ARG
1	D	463	LEU
1	D	470	MET
2	F	566	LEU
2	G	553	VAL
2	H	553	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	216	HIS
1	B	483	HIS
1	C	216	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	165/211 (78%)	0.13	2 (1%) 81 55	54, 92, 138, 165	0
1	B	165/211 (78%)	0.12	2 (1%) 81 55	54, 92, 138, 174	0
1	C	164/211 (77%)	0.23	4 (2%) 62 32	56, 107, 168, 200	0
1	D	164/211 (77%)	0.33	6 (3%) 45 19	58, 107, 167, 200	0
2	E	39/56 (69%)	-0.04	1 (2%) 59 29	55, 80, 140, 148	0
2	F	36/56 (64%)	0.08	0 100 100	56, 78, 120, 133	0
2	G	29/56 (51%)	0.21	1 (3%) 49 21	64, 82, 130, 151	0
2	H	29/56 (51%)	0.09	0 100 100	70, 88, 138, 161	0
All	All	791/1068 (74%)	0.18	16 (2%) 68 39	54, 96, 154, 200	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	503	ALA	4.4
1	D	442	ASP	3.5
1	A	288	SER	3.3
2	G	568	ILE	2.9
1	B	440	GLU	2.7
2	E	566	LEU	2.7
1	D	498	PHE	2.5
1	D	184	LEU	2.4
1	C	197	LEU	2.4
1	D	441	PHE	2.4
1	B	450	ILE	2.2
1	C	192	ASN	2.2
1	C	191	ILE	2.2
1	A	191	ILE	2.1
1	C	193	ARG	2.1
1	D	286	THR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.