Full wwPDB X-ray Structure Validation Report (i)

Aug 19, 2024 – 04:10 PM JST

PDB ID	:	8WHH
Title	:	Crystal structure of Se-Met derivative CLASP2 in complex with CLIP170
Authors	:	Jin, G.; Wei, Z.
Deposited on	:	2023-09-23
Resolution	:	3.80 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 (1)) were used in the production of this report:

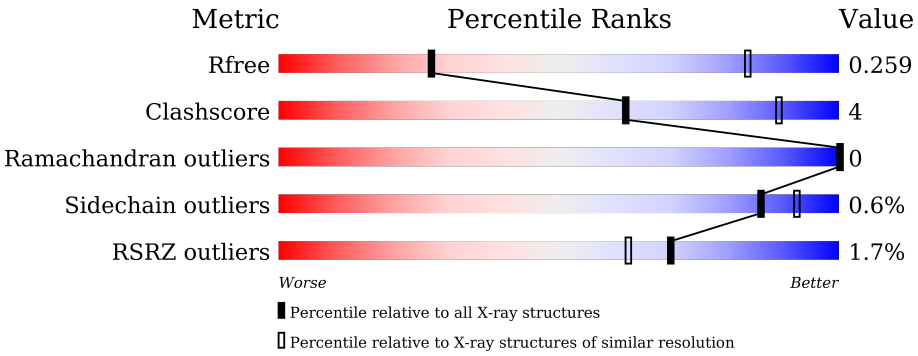
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	235	77% 17% 6%
1	B	235	% 77% 17% 7%
1	C	235	3% 78% 15% 7%
1	D	235	4% 80% 13% 7%
2	E	111	91% 7%
2	F	111	% 90% 8%

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Mol	Chain	Length	Quality of chain
2	G	111	
2	H	111	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10075 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 CLIP-associating protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	Se	0	0	0
			1694	1080	291	314	4	5			
1	B	219	Total	C	N	O	S	Se	0	0	0
			1685	1075	288	313	4	5			
1	C	219	Total	C	N	O	S	Se	0	0	0
			1695	1081	292	313	4	5			
1	D	219	Total	C	N	O	S	Se	0	0	0
			1690	1078	292	311	4	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1245	GLY	-	expression tag	UNP O75122
A	1246	PRO	-	expression tag	UNP O75122
A	1247	GLY	-	expression tag	UNP O75122
A	1248	SER	-	expression tag	UNP O75122
A	1249	GLU	-	expression tag	UNP O75122
A	1250	PHE	-	expression tag	UNP O75122
B	1245	GLY	-	expression tag	UNP O75122
B	1246	PRO	-	expression tag	UNP O75122
B	1247	GLY	-	expression tag	UNP O75122
B	1248	SER	-	expression tag	UNP O75122
B	1249	GLU	-	expression tag	UNP O75122
B	1250	PHE	-	expression tag	UNP O75122
C	1245	GLY	-	expression tag	UNP O75122
C	1246	PRO	-	expression tag	UNP O75122
C	1247	GLY	-	expression tag	UNP O75122
C	1248	SER	-	expression tag	UNP O75122
C	1249	GLU	-	expression tag	UNP O75122
C	1250	PHE	-	expression tag	UNP O75122
D	1245	GLY	-	expression tag	UNP O75122
D	1246	PRO	-	expression tag	UNP O75122
D	1247	GLY	-	expression tag	UNP O75122

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1248	SER	-	expression tag	UNP O75122
D	1249	GLU	-	expression tag	UNP O75122
D	1250	PHE	-	expression tag	UNP O75122

- Molecule 2 is a protein called CLIP1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	103	Total	C	N	O	S	0	0	0
			834	508	149	175	2			
2	F	102	Total	C	N	O	S	0	0	0
			817	498	144	173	2			
2	G	105	Total	C	N	O	S	0	0	0
			843	513	151	177	2			
2	H	103	Total	C	N	O	S	0	0	0
			817	498	145	172	2			

There are 16 discrepancies between the modelled and reference sequences:

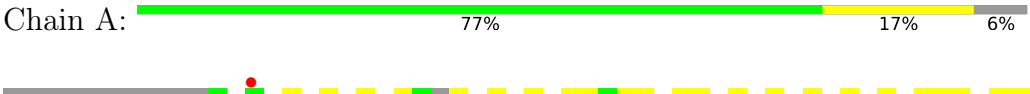
Chain	Residue	Modelled	Actual	Comment	Reference
E	346	GLY	-	expression tag	UNP Q6P5Z9
E	347	PRO	-	expression tag	UNP Q6P5Z9
E	348	GLY	-	expression tag	UNP Q6P5Z9
E	349	SER	-	expression tag	UNP Q6P5Z9
F	346	GLY	-	expression tag	UNP Q6P5Z9
F	347	PRO	-	expression tag	UNP Q6P5Z9
F	348	GLY	-	expression tag	UNP Q6P5Z9
F	349	SER	-	expression tag	UNP Q6P5Z9
G	346	GLY	-	expression tag	UNP Q6P5Z9
G	347	PRO	-	expression tag	UNP Q6P5Z9
G	348	GLY	-	expression tag	UNP Q6P5Z9
G	349	SER	-	expression tag	UNP Q6P5Z9
H	346	GLY	-	expression tag	UNP Q6P5Z9
H	347	PRO	-	expression tag	UNP Q6P5Z9
H	348	GLY	-	expression tag	UNP Q6P5Z9
H	349	SER	-	expression tag	UNP Q6P5Z9

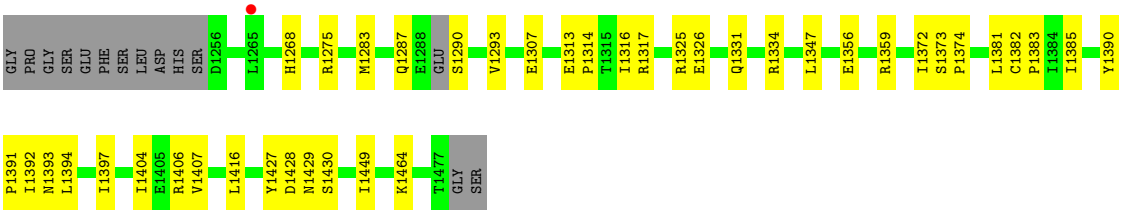
3 Residue-property plots (i)

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: CLIP-associating protein 2

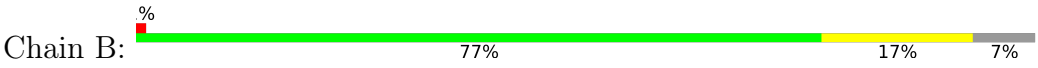
Chain A:

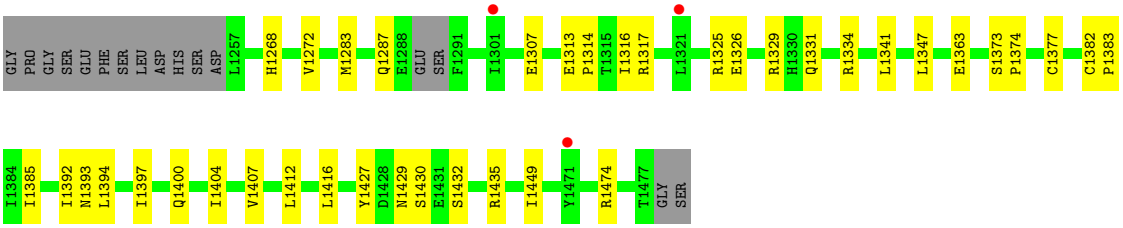




• Molecule 1: CLIP-associating protein 2

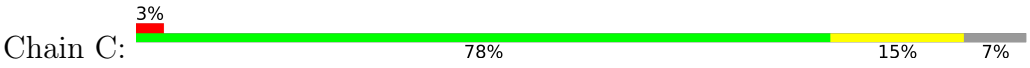
Chain B:

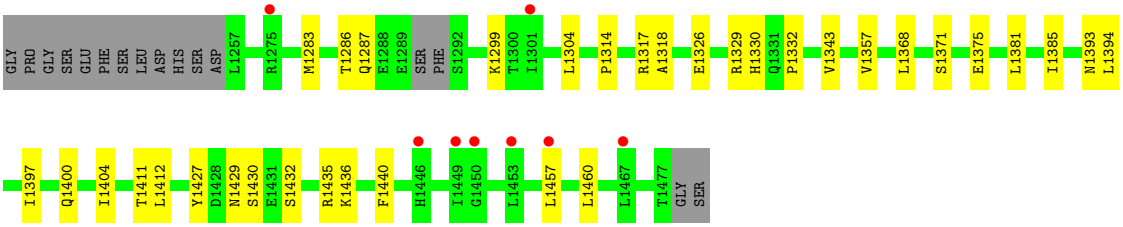




• Molecule 1: CLIP-associating protein 2

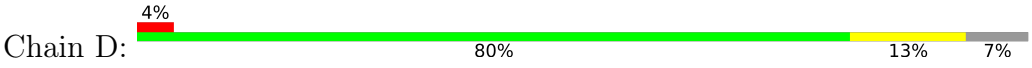
Chain C:

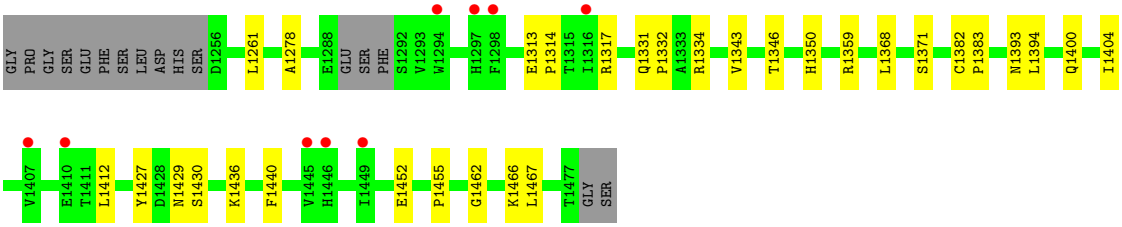




• Molecule 1: CLIP-associating protein 2

Chain D:



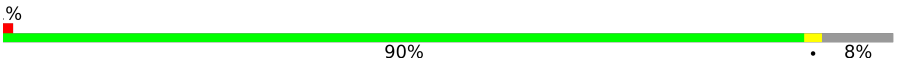


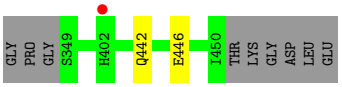
• Molecule 2: CLIP1 protein

Chain E:

• Molecule 2: CLIP1 protein

Chain F:





• Molecule 2: CLIP1 protein

Chain G:

• Molecule 2: CLIP1 protein

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.11Å 100.83Å 226.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 3.80 49.43 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.43-3.80) 90.6 (49.43-3.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.217 , 0.266 0.217 , 0.259	Depositor DCC
R_{free} test set	1002 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	134.7	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 123.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10075	wwPDB-VP
Average B, all atoms (Å^2)	174.0	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 33.16 % 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 8.3625e-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

5.1 Standard geometry

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	0/1713	0.49	0/2318
1	B	0.29	0/1704	0.50	0/2306
1	C	0.24	0/1714	0.44	0/2317
1	D	0.28	0/1709	0.45	0/2311
2	E	0.29	0/838	0.41	0/1123
2	F	0.29	0/821	0.41	0/1102
2	G	0.27	0/847	0.40	0/1135
2	H	0.29	0/821	0.42	0/1102
All	All	0.28	0/10167	0.45	0/13714

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

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	1694	0	1727	23	0
1	B	1685	0	1721	21	0
1	C	1695	0	1743	21	0
1	D	1690	0	1737	19	0
2	E	834	0	825	2	0
2	F	817	0	796	1	0
2	G	843	0	830	2	0
2	H	817	0	795	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10075	0	10174	89	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 4.

All (89) 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:C:1314:PRO:HA	1:C:1317:ARG:HE	1.59	0.68
2:E:446:GLU:OE2	1:B:1474:ARG:NH2	2.25	0.66
1:B:1347:LEU:HB3	1:B:1392:ILE:HG23	1.81	0.62
1:B:1325:ARG:NH1	1:B:1363:GLU:OE1	2.33	0.62
1:B:1314:PRO:HA	1:B:1317:ARG:HE	1.65	0.60
1:A:1347:LEU:HB3	1:A:1392:ILE:HG23	1.82	0.60
1:A:1290:SER:HB2	1:A:1293:VAL:HG23	1.84	0.60
1:B:1385:ILE:HD12	1:B:1397:ILE:HG13	1.84	0.60
1:D:1314:PRO:HA	1:D:1317:ARG:HE	1.68	0.59
1:D:1436:LYS:NZ	2:H:439:GLU:HG3	2.18	0.58
1:A:1314:PRO:HA	1:A:1317:ARG:HE	1.70	0.57
1:C:1343:VAL:HG22	1:C:1368:LEU:HD21	1.87	0.57
1:A:1429:ASN:OD1	1:A:1430:SER:N	2.38	0.57
1:A:1275:ARG:HH12	1:A:1316:ILE:HG21	1.70	0.56
1:B:1416:LEU:HD11	1:B:1449:ILE:HD13	1.87	0.56
1:B:1268:HIS:NE2	1:B:1307:GLU:OE1	2.30	0.55
2:H:432:GLU:OE2	2:H:436:ARG:NH2	2.40	0.55
1:A:1331:GLN:OE1	1:A:1334:ARG:NH1	2.41	0.54
1:B:1429:ASN:OD1	1:B:1430:SER:N	2.40	0.54
1:B:1283:MSE:HE3	1:B:1326:GLU:HG3	1.90	0.53
1:A:1372:ILE:O	1:A:1406:ARG:NH2	2.42	0.53
1:C:1318:ALA:HB2	1:C:1357:VAL:HG22	1.92	0.52
1:C:1332:PRO:HB3	1:C:1371:SER:HB3	1.91	0.52
1:A:1283:MSE:O	1:A:1287:GLN:HG2	2.09	0.52
1:D:1436:LYS:HZ3	2:H:439:GLU:HG3	1.75	0.52
1:A:1356:GLU:HG3	1:A:1359:ARG:HH11	1.73	0.51
1:C:1400:GLN:O	1:C:1404:ILE:HG12	2.09	0.51
1:C:1375:GLU:HG2	1:C:1411:THR:HG21	1.93	0.51
1:D:1400:GLN:O	1:D:1404:ILE:HG12	2.11	0.51
1:D:1261:LEU:HD22	1:D:1278:ALA:HA	1.93	0.50
1:C:1432:SER:HA	1:C:1435:ARG:HE	1.76	0.50
1:A:1428:ASP:OD1	1:A:1464:LYS:NZ	2.37	0.50
1:B:1283:MSE:O	1:B:1287:GLN:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1429:ASN:OD1	1:D:1430:SER:N	2.45	0.49
1:A:1404:ILE:O	1:A:1407:VAL:HG22	2.12	0.49
1:D:1404:ILE:HD12	1:D:1412:LEU:HD13	1.94	0.49
1:B:1404:ILE:HD12	1:B:1412:LEU:HD13	1.94	0.49
1:D:1332:PRO:HB3	1:D:1371:SER:HB3	1.94	0.49
1:B:1272:VAL:HG13	1:B:1316:ILE:HD11	1.95	0.48
1:A:1416:LEU:HD11	1:A:1449:ILE:HD13	1.95	0.48
1:C:1314:PRO:HB3	1:C:1317:ARG:HH21	1.78	0.48
1:D:1359:ARG:HH12	2:H:432:GLU:HB2	1.79	0.48
1:B:1432:SER:HA	1:B:1435:ARG:HE	1.78	0.48
1:C:1385:ILE:HD12	1:C:1397:ILE:HG13	1.95	0.48
1:C:1404:ILE:HD12	1:C:1412:LEU:HD13	1.95	0.47
1:A:1385:ILE:HD12	1:A:1397:ILE:HG13	1.96	0.47
2:F:442:GLN:O	2:F:446:GLU:HG2	2.15	0.47
1:A:1325:ARG:NH2	1:A:1326:GLU:OE2	2.48	0.47
1:B:1393:ASN:OD1	1:B:1394:LEU:N	2.48	0.47
1:C:1381:LEU:O	1:C:1385:ILE:HG12	2.16	0.47
1:C:1436:LYS:HE2	1:C:1440:PHE:CZ	2.51	0.46
1:A:1268:HIS:NE2	1:A:1307:GLU:OE1	2.48	0.46
1:C:1326:GLU:OE1	1:C:1329:ARG:NH1	2.43	0.46
1:D:1331:GLN:OE1	1:D:1334:ARG:NE	2.31	0.46
1:A:1382:CYS:HB2	1:A:1383:PRO:HD3	1.98	0.45
1:B:1331:GLN:OE1	1:B:1334:ARG:NH1	2.50	0.45
1:B:1400:GLN:O	1:B:1404:ILE:HG12	2.17	0.45
1:C:1429:ASN:OD1	1:C:1430:SER:N	2.50	0.45
1:A:1381:LEU:O	1:A:1385:ILE:HG12	2.17	0.45
1:A:1356:GLU:HG3	1:A:1359:ARG:NH1	2.31	0.44
2:H:442:GLN:O	2:H:446:GLU:HG2	2.17	0.44
1:D:1393:ASN:OD1	1:D:1394:LEU:N	2.50	0.44
1:B:1373:SER:HA	1:B:1374:PRO:HD3	1.80	0.44
1:A:1283:MSE:HE3	1:A:1326:GLU:HG3	1.98	0.44
1:B:1382:CYS:HB2	1:B:1383:PRO:HD3	2.00	0.44
1:C:1393:ASN:OD1	1:C:1394:LEU:N	2.50	0.43
1:B:1341:LEU:HB2	2:G:390:GLN:HB3	2.00	0.43
1:D:1313:GLU:HA	1:D:1314:PRO:HD2	1.89	0.43
1:C:1283:MSE:O	1:C:1287:GLN:HG2	2.18	0.43
1:C:1286:THR:HG22	1:C:1330:HIS:ND1	2.34	0.42
2:E:427:LEU:HD23	2:E:427:LEU:HA	1.91	0.42
1:C:1304:LEU:HD23	1:C:1304:LEU:HA	1.87	0.42
1:A:1390:TYR:HA	1:A:1391:PRO:HA	1.82	0.42
1:B:1313:GLU:HA	1:B:1314:PRO:HD2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1299:LYS:HB2	2:H:401:GLN:NE2	2.35	0.42
1:C:1457:LEU:HD22	1:C:1460:LEU:HD11	2.02	0.42
1:D:1462:GLY:O	1:D:1466:LYS:HG3	2.19	0.42
1:D:1382:CYS:HB2	1:D:1383:PRO:HD3	2.02	0.41
1:D:1452:GLU:O	1:D:1455:PRO:HD2	2.21	0.41
1:D:1436:LYS:HE2	1:D:1440:PHE:CE2	2.55	0.41
1:A:1393:ASN:OD1	1:A:1394:LEU:N	2.54	0.41
2:G:447:GLU:O	2:G:451:THR:HG23	2.21	0.41
1:A:1373:SER:HA	1:A:1374:PRO:HD3	1.77	0.41
1:D:1343:VAL:HG22	1:D:1368:LEU:HD21	2.02	0.41
1:B:1404:ILE:O	1:B:1407:VAL:HG22	2.20	0.40
1:D:1467:LEU:HA	2:H:450:ILE:HD13	2.02	0.40
1:A:1313:GLU:HA	1:A:1314:PRO:HD3	1.91	0.40
1:D:1346:THR:HG22	1:D:1350:HIS:HE1	1.86	0.40
1:C:1404:ILE:HD13	1:C:1404:ILE:HA	1.92	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	217/235 (92%)	217 (100%)	0	0	100	100
1	B	215/235 (92%)	214 (100%)	1 (0%)	0	100	100
1	C	215/235 (92%)	215 (100%)	0	0	100	100
1	D	215/235 (92%)	214 (100%)	1 (0%)	0	100	100
2	E	101/111 (91%)	101 (100%)	0	0	100	100
2	F	100/111 (90%)	100 (100%)	0	0	100	100
2	G	103/111 (93%)	103 (100%)	0	0	100	100
2	H	101/111 (91%)	101 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1267/1384 (92%)	1265 (100%)	2 (0%)	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	183/204 (90%)	182 (100%)	1 (0%)	88 94
1	B	183/204 (90%)	180 (98%)	3 (2%)	62 79
1	C	185/204 (91%)	184 (100%)	1 (0%)	88 94
1	D	184/204 (90%)	183 (100%)	1 (0%)	88 94
2	E	90/95 (95%)	90 (100%)	0	100 100
2	F	87/95 (92%)	87 (100%)	0	100 100
2	G	90/95 (95%)	90 (100%)	0	100 100
2	H	86/95 (90%)	86 (100%)	0	100 100
All	All	1088/1196 (91%)	1082 (99%)	6 (1%)	86 92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1427	TYR
1	B	1329	ARG
1	B	1377	CYS
1	B	1427	TYR
1	C	1427	TYR
1	D	1427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	216/235 (91%)	-0.12	1 (0%) 91 87	83, 143, 239, 299	0
1	B	214/235 (91%)	-0.04	3 (1%) 75 68	81, 142, 239, 336	0
1	C	214/235 (91%)	-0.05	8 (3%) 41 34	131, 202, 275, 350	0
1	D	214/235 (91%)	0.10	9 (4%) 36 30	128, 204, 276, 322	0
2	E	103/111 (92%)	-0.28	0 100 100	105, 152, 202, 233	0
2	F	102/111 (91%)	-0.15	1 (0%) 82 76	103, 165, 215, 239	0
2	G	105/111 (94%)	-0.26	0 100 100	128, 157, 206, 282	0
2	H	103/111 (92%)	-0.20	0 100 100	118, 169, 213, 270	0
All	All	1271/1384 (91%)	-0.09	22 (1%) 70 62	81, 170, 255, 350	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1446	HIS	3.5
1	D	1449	ILE	3.2
1	C	1467	LEU	2.6
1	D	1316	ILE	2.6
1	D	1445	VAL	2.6
2	F	402	HIS	2.5
1	C	1453	LEU	2.4
1	C	1449	ILE	2.4
1	D	1298	PHE	2.3
1	C	1275	ARG	2.3
1	D	1294	TRP	2.3
1	D	1297	HIS	2.3
1	C	1450	GLY	2.3
1	C	1301	ILE	2.2
1	C	1457	LEU	2.2
1	D	1407	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1265	LEU	2.2
1	B	1301	ILE	2.1
1	C	1446	HIS	2.1
1	D	1410	GLU	2.1
1	B	1471	TYR	2.1
1	B	1321	LEU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.