



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:08 am BST

PDB ID : 4XH9
Title : CRYSTAL STRUCTURE OF HUMAN RHOA IN COMPLEX WITH DH/PH
FRAGMENT OF THE GUANINE NUCLEOTIDE EXCHANGE FACTOR
NET1
Authors : Garcia, C.; Petit, P.; Boutin, J.A.; Ferry, G.; Vuillard, L.
Deposited on : 2015-01-05
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

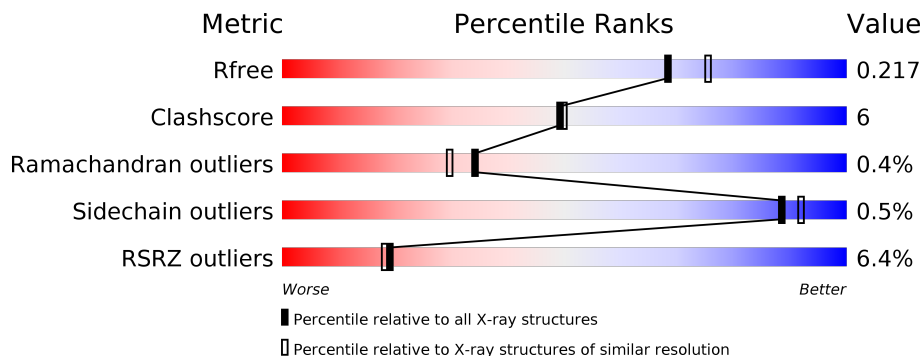
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	361	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">9% 77% 16% • 7%</p>
1	D	361	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">6% 81% 11% • 6%</p>
2	B	180	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">4% 87% 10% •</p>
2	E	180	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">3% 89% 7% ••</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9206 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 Neuroepithelial cell-transforming gene 1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	336	Total 2753	C 1751	N 487	O 504	S 11	0	0	0
1	D	338	Total 2784	C 1769	N 497	O 508	S 10	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	MET	-	initiating methionine	UNP Q7Z628
A	148	GLY	-	expression tag	UNP Q7Z628
A	502	HIS	-	expression tag	UNP Q7Z628
A	503	HIS	-	expression tag	UNP Q7Z628
A	504	HIS	-	expression tag	UNP Q7Z628
A	505	HIS	-	expression tag	UNP Q7Z628
A	506	HIS	-	expression tag	UNP Q7Z628
A	507	HIS	-	expression tag	UNP Q7Z628
D	147	MET	-	initiating methionine	UNP Q7Z628
D	148	GLY	-	expression tag	UNP Q7Z628
D	502	HIS	-	expression tag	UNP Q7Z628
D	503	HIS	-	expression tag	UNP Q7Z628
D	504	HIS	-	expression tag	UNP Q7Z628
D	505	HIS	-	expression tag	UNP Q7Z628
D	506	HIS	-	expression tag	UNP Q7Z628
D	507	HIS	-	expression tag	UNP Q7Z628

- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	174	Total 1374	C 865	N 234	O 265	S 10	0	0	0
2	E	174	Total 1374	C 865	N 234	O 265	S 10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP P61586
B	25	ASN	PHE	engineered mutation	UNP P61586
E	1	GLY	-	expression tag	UNP P61586
E	25	ASN	PHE	engineered mutation	UNP P61586

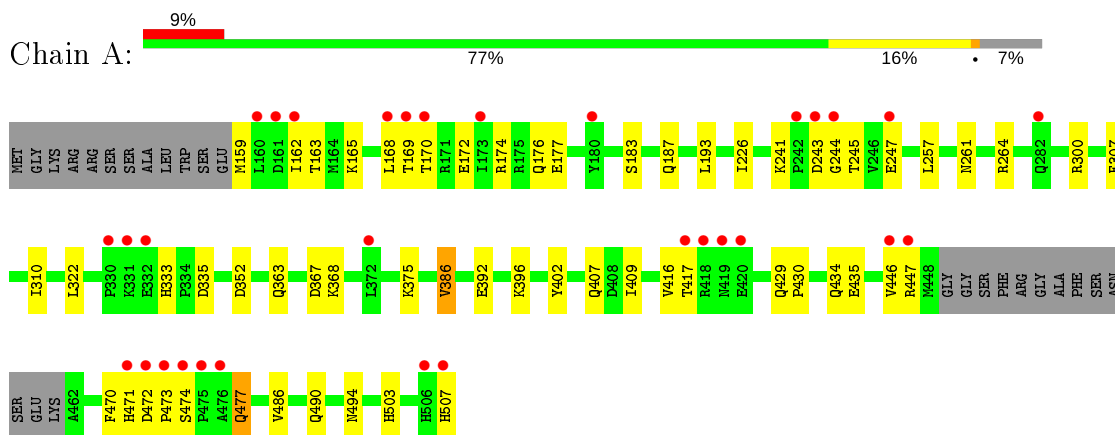
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	337	Total O 337 337	0	0
3	B	170	Total O 170 170	0	0
3	D	291	Total O 291 291	0	0
3	E	123	Total O 123 123	0	0

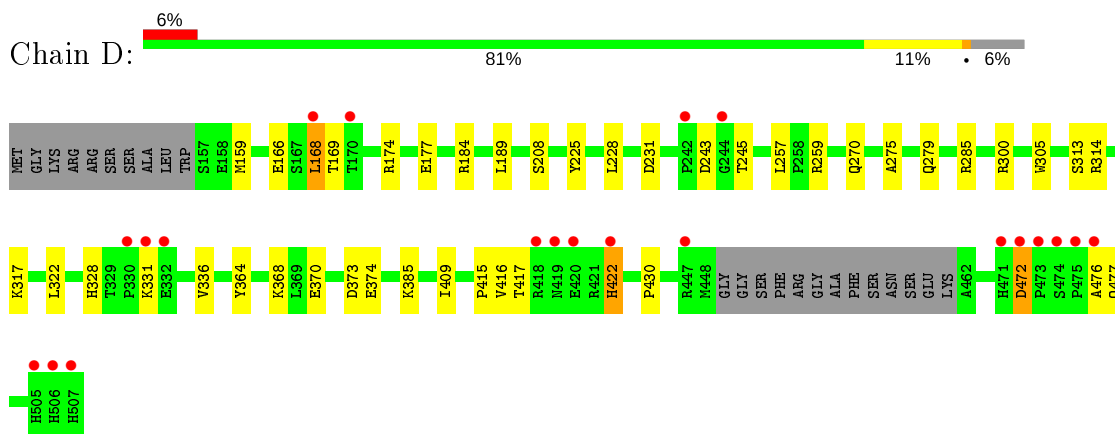
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

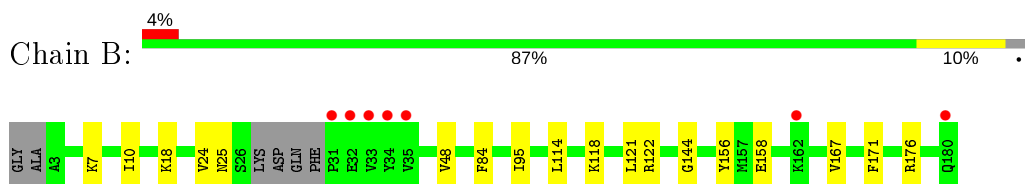
- Molecule 1: Neuroepithelial cell-transforming gene 1 protein




- Molecule 1: Neuroepithelial cell-transforming gene 1 protein



- Molecule 2: Transforming protein RhoA



- Molecule 2: Transforming protein RhoA

Chain E:  3% 89% 7% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.10Å 101.40Å 116.20Å 90.00° 94.30° 90.00°	Depositor
Resolution (Å)	34.69 – 2.00 34.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.69-2.00) 99.4 (34.69-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.189 , 0.217 0.190 , 0.217	Depositor DCC
R_{free} test set	4195 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtrriage
Anisotropy	0.330	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9206	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.28	0/2813	0.45	0/3803
1	D	0.27	0/2850	0.46	0/3851
2	B	0.27	0/1399	0.46	0/1890
2	E	0.34	0/1399	0.47	0/1890
All	All	0.28	0/8461	0.46	0/11434

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	472	ASP	Peptide
2	E	33	VAL	Peptide

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	2753	0	2745	45	0
1	D	2784	0	2782	32	0
2	B	1374	0	1368	13	0
2	E	1374	0	1368	11	0
3	A	337	0	0	6	0
3	B	170	0	0	5	0
3	D	291	0	0	5	0
3	E	123	0	0	0	0
All	All	9206	0	8263	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (98) 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:A:241:LYS:NZ	1:A:247:GLU:OE2	2.02	0.92
1:A:392:GLU:OE1	3:A:601:HOH:O	1.97	0.82
1:A:429:GLN:H	1:A:477:GLN:HE22	1.30	0.79
1:A:300:ARG:NH1	3:A:694:HOH:O	2.18	0.76
1:A:470:PHE:CD1	1:A:477:GLN:HG2	2.22	0.75
2:E:122:ARG:NH2	2:E:158:GLU:OE1	2.19	0.71
1:D:416:VAL:HG12	1:D:417:THR:N	2.05	0.69
1:D:177:GLU:HG3	2:E:34:TYR:CE2	2.27	0.69
1:D:300:ARG:NH1	3:D:780:HOH:O	2.25	0.69
1:D:177:GLU:HG3	2:E:34:TYR:CZ	2.29	0.68
2:B:122:ARG:NH2	2:B:158:GLU:OE1	2.26	0.67
1:A:368:LYS:NZ	3:A:894:HOH:O	2.28	0.66
2:B:118:LYS:HB3	2:B:121:LEU:HD13	1.78	0.65
1:A:375:LYS:NZ	3:A:898:HOH:O	2.29	0.64
2:B:25:ASN:ND2	2:B:171:PHE:CD2	2.66	0.64
1:A:170:THR:O	1:A:174:ARG:HG3	2.00	0.62
1:D:189:LEU:HD22	1:D:314:ARG:HG2	1.83	0.61
1:A:243:ASP:HB3	1:A:245:THR:HG23	1.82	0.61
2:E:24:VAL:HG23	2:E:167:VAL:HG11	1.83	0.61
1:A:503:HIS:O	1:A:507:HIS:N	2.34	0.60
1:D:168:LEU:HD13	1:D:169:THR:H	1.66	0.60
2:E:125:GLU:HB3	2:E:129:ARG:NH2	2.17	0.60
1:A:168:LEU:HD12	1:A:169:THR:H	1.67	0.59
1:A:168:LEU:HD23	1:A:172:GLU:HG2	1.85	0.59
1:A:471:HIS:ND1	1:A:473:PRO:HG2	2.18	0.59
1:A:163:THR:HG22	1:A:165:LYS:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ARG:NH2	3:D:716:HOH:O	2.30	0.59
1:A:264:ARG:NE	1:A:352:ASP:OD2	2.36	0.58
1:A:241:LYS:HE3	1:A:247:GLU:HG3	1.84	0.58
1:D:416:VAL:HG12	1:D:417:THR:H	1.68	0.58
1:A:470:PHE:CE1	1:A:477:GLN:HG2	2.39	0.57
2:E:118:LYS:HB3	2:E:121:LEU:HD13	1.85	0.57
1:D:231:ASP:OD2	1:D:259:ARG:NH1	2.39	0.56
1:D:257:LEU:HD11	1:D:322:LEU:HD21	1.89	0.54
1:D:331:LYS:HA	1:D:336:VAL:HG21	1.88	0.54
1:D:275:ALA:O	1:D:279:GLN:HG3	2.09	0.53
2:B:84:PHE:HB3	2:B:95:ILE:HD11	1.90	0.53
2:B:10:ILE:HG12	2:B:18:LYS:HG2	1.91	0.52
2:B:176:ARG:NH1	3:B:203:HOH:O	2.41	0.51
1:D:177:GLU:OE1	1:D:177:GLU:HA	2.11	0.51
1:D:184:ARG:NH1	3:D:850:HOH:O	2.44	0.51
1:D:208:SER:O	1:D:285:ARG:NH2	2.43	0.51
1:D:417:THR:CG2	1:D:422:HIS:CE1	2.94	0.50
2:B:7:LYS:NZ	3:B:243:HOH:O	2.44	0.50
1:A:162:ILE:HD12	1:A:244:GLY:HA3	1.94	0.50
1:A:477:GLN:HG3	1:A:477:GLN:O	2.12	0.50
1:A:159:MET:HE2	1:A:177:GLU:HG2	1.93	0.49
1:A:470:PHE:HD1	1:A:477:GLN:HG2	1.76	0.49
1:A:193:LEU:HB2	1:A:226:ILE:HD11	1.95	0.49
1:A:490:GLN:HG2	3:B:207:HOH:O	2.13	0.49
2:E:32:GLU:O	2:E:33:VAL:HG12	2.13	0.48
1:D:417:THR:HG22	1:D:422:HIS:CE1	2.47	0.48
1:A:257:LEU:HD11	1:A:322:LEU:HD21	1.94	0.48
1:D:476:ALA:O	1:D:477:GLN:NE2	2.47	0.48
1:A:392:GLU:HG2	1:A:402:TYR:CD2	2.49	0.48
1:A:486:VAL:HG23	3:A:780:HOH:O	2.13	0.48
1:A:434:GLN:HA	1:A:503:HIS:CD2	2.48	0.47
1:A:470:PHE:HB3	1:A:474:SER:OG	2.14	0.47
1:D:416:VAL:CG1	1:D:417:THR:N	2.76	0.47
2:E:142:GLU:HG3	2:E:145:ARG:NH2	2.30	0.47
2:B:25:ASN:ND2	2:B:171:PHE:CG	2.81	0.47
1:A:386:VAL:HG13	1:A:407:GLN:HB2	1.96	0.47
1:D:370:GLU:OE2	3:D:875:HOH:O	2.20	0.46
1:A:363:GLN:NE2	1:A:367:ASP:OD1	2.45	0.46
1:D:243:ASP:HB3	1:D:245:THR:H	1.81	0.46
1:A:471:HIS:ND1	1:A:473:PRO:HD2	2.30	0.46
1:D:313:SER:OG	1:D:317:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:33:VAL:O	2:E:34:TYR:CG	2.69	0.46
1:A:183:SER:O	1:A:187:GLN:HG3	2.17	0.45
2:B:24:VAL:HG23	2:B:167:VAL:HG11	2.00	0.44
1:D:174:ARG:HE	1:D:328:HIS:CE1	2.36	0.44
1:D:225:TYR:O	1:D:228:LEU:HB3	2.16	0.44
1:A:435:GLU:O	1:A:471:HIS:N	2.45	0.44
2:B:95:ILE:HD13	2:B:114:LEU:HD11	2.00	0.43
1:A:490:GLN:HG3	1:A:494:ASN:ND2	2.33	0.43
1:D:270:GLN:HG2	1:D:305:TRP:CH2	2.54	0.43
1:D:364:TYR:O	1:D:368:LYS:HG3	2.19	0.43
1:D:373:ASP:OD1	1:D:374:GLU:N	2.51	0.43
1:A:241:LYS:NZ	1:A:247:GLU:CD	2.72	0.42
1:D:417:THR:HG22	1:D:422:HIS:ND1	2.34	0.42
2:B:176:ARG:NH2	3:B:206:HOH:O	2.51	0.42
1:A:300:ARG:NE	3:A:869:HOH:O	2.35	0.42
1:A:261:ASN:O	1:A:264:ARG:HG3	2.20	0.42
1:D:159:MET:SD	2:E:34:TYR:CE2	3.12	0.42
1:A:416:VAL:HG12	1:A:417:THR:O	2.20	0.42
1:D:415:PRO:HB3	1:D:422:HIS:CD2	2.55	0.42
1:A:310:ILE:HD13	1:A:310:ILE:HA	1.84	0.41
1:A:409:ILE:HD11	1:A:430:PRO:HB2	2.02	0.41
1:D:409:ILE:HD11	1:D:430:PRO:HB2	2.02	0.41
1:A:396:LYS:HD3	1:A:446:VAL:CG1	2.51	0.41
2:B:48:VAL:HG12	3:B:223:HOH:O	2.20	0.41
1:A:307:PHE:HA	1:A:310:ILE:HG12	2.03	0.41
1:D:385:LYS:NZ	3:D:610:HOH:O	2.53	0.41
1:A:172:GLU:OE2	1:A:176:GLN:NE2	2.54	0.40
1:A:241:LYS:C	1:A:243:ASP:N	2.74	0.40
2:E:168:ARG:HB2	2:E:168:ARG:HE	1.69	0.40
2:B:144:GLY:HA3	2:B:156:TYR:CZ	2.55	0.40
1:A:333:HIS:ND1	1:A:335:ASP:HB2	2.37	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	332/361 (92%)	321 (97%)	10 (3%)	1 (0%)	41	37
1	D	336/361 (93%)	328 (98%)	6 (2%)	2 (1%)	25	19
2	B	170/180 (94%)	168 (99%)	2 (1%)	0	100	100
2	E	170/180 (94%)	164 (96%)	5 (3%)	1 (1%)	25	19
All	All	1008/1082 (93%)	981 (97%)	23 (2%)	4 (0%)	34	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	ASP
1	D	472	ASP
1	D	166	GLU
2	E	33	VAL

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	304/328 (93%)	301 (99%)	3 (1%)	76	81
1	D	307/328 (94%)	305 (99%)	2 (1%)	84	88
2	B	152/156 (97%)	152 (100%)	0	100	100
2	E	152/156 (97%)	152 (100%)	0	100	100
All	All	915/968 (94%)	910 (100%)	5 (0%)	88	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	386	VAL
1	A	447	ARG
1	A	477	GLN
1	D	168	LEU

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Mol	Chain	Res	Type
1	D	422	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	477	GLN
2	E	52	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	336/361 (93%)	0.17	31 (9%) 9 8	16, 29, 69, 81	0
1	D	338/361 (93%)	0.09	21 (6%) 20 19	18, 31, 67, 80	0
2	B	174/180 (96%)	0.05	7 (4%) 38 37	14, 29, 57, 121	0
2	E	174/180 (96%)	-0.10	6 (3%) 45 44	16, 31, 60, 122	0
All	All	1022/1082 (94%)	0.08	65 (6%) 19 18	14, 30, 67, 122	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	34	TYR	10.9
1	D	473	PRO	9.1
2	B	33	VAL	8.9
2	E	33	VAL	8.8
1	D	474	SER	8.2
1	A	473	PRO	7.6
1	A	474	SER	7.3
2	E	31	PRO	6.1
2	B	31	PRO	5.9
2	B	34	TYR	5.5
1	A	160	LEU	5.5
1	A	420	GLU	5.3
1	A	471	HIS	5.2
1	A	475	PRO	5.1
1	D	168	LEU	4.9
1	D	447	ARG	4.9
1	D	475	PRO	4.6
1	A	472	ASP	4.5
2	E	32	GLU	4.5
1	A	417	THR	4.3
1	A	168	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	32	GLU	4.0
2	E	26	SER	4.0
1	A	447	ARG	4.0
1	A	418	ARG	3.9
1	D	422	HIS	3.6
1	D	507	HIS	3.5
1	D	418	ARG	3.4
2	B	35	VAL	3.3
1	A	243	ASP	3.3
1	D	506	HIS	3.2
1	A	331	LYS	3.2
1	D	420	GLU	3.2
1	A	161	ASP	3.1
1	D	244	GLY	3.0
1	A	162	ILE	2.9
1	D	472	ASP	2.9
1	D	419	ASN	2.9
1	A	476	ALA	2.8
1	A	330	PRO	2.8
1	A	282	GLN	2.7
1	D	476	ALA	2.7
1	A	332	GLU	2.7
1	D	331	LYS	2.6
1	A	507	HIS	2.6
1	A	173	ILE	2.6
1	D	471	HIS	2.5
1	D	170	THR	2.5
1	D	242	PRO	2.5
1	A	419	ASN	2.5
1	A	170	THR	2.4
1	D	505	HIS	2.4
2	B	180	GLN	2.4
1	A	169	THR	2.4
2	E	24	VAL	2.4
2	B	162	LYS	2.4
1	A	372	LEU	2.3
1	A	244	GLY	2.3
1	D	330	PRO	2.3
1	A	247	GLU	2.3
1	D	332	GLU	2.3
1	A	242	PRO	2.2
1	A	180	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	446	VAL	2.1
1	A	506	HIS	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 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.