Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:57 PM GMT

PDB ID	:	3SAH
Title	:	Crystal structure of the human RRP6 catalytic domain with Y436A mutation in the catalytic site
Authors	:	Januszyk, K.; Liu, Q.; Lima, C.D.
Deposited on	:	2011-06-02
Resolution	:	2.65 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

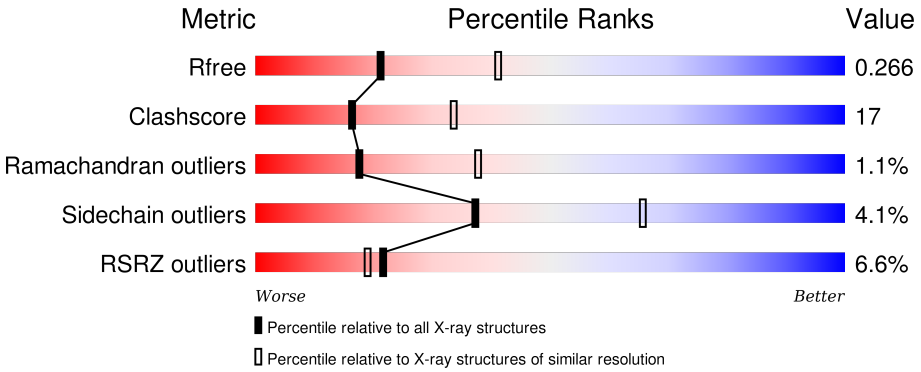
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 <=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	428	7%, 57%, 30%, ·, 12%
1	B	428	4%, 58%, 29%, ·, 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	B	2	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6506 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 Exosome component 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3133	2006	540	569	18			
1	B	382	Total	C	N	O	S	0	0	0
			3166	2026	548	574	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	SER	-	EXPRESSION TAG	UNP Q01780
A	436	ALA	TYR	ENGINEERED MUTATION	UNP Q01780
B	179	SER	-	EXPRESSION TAG	UNP Q01780
B	436	ALA	TYR	ENGINEERED MUTATION	UNP Q01780

- Molecule 2 is YTTRIUM (III) ION (three-letter code: YT3) (formula: Y).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Y	0	0
			1	1		
2	A	2	Total	Y	0	0
			2	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		

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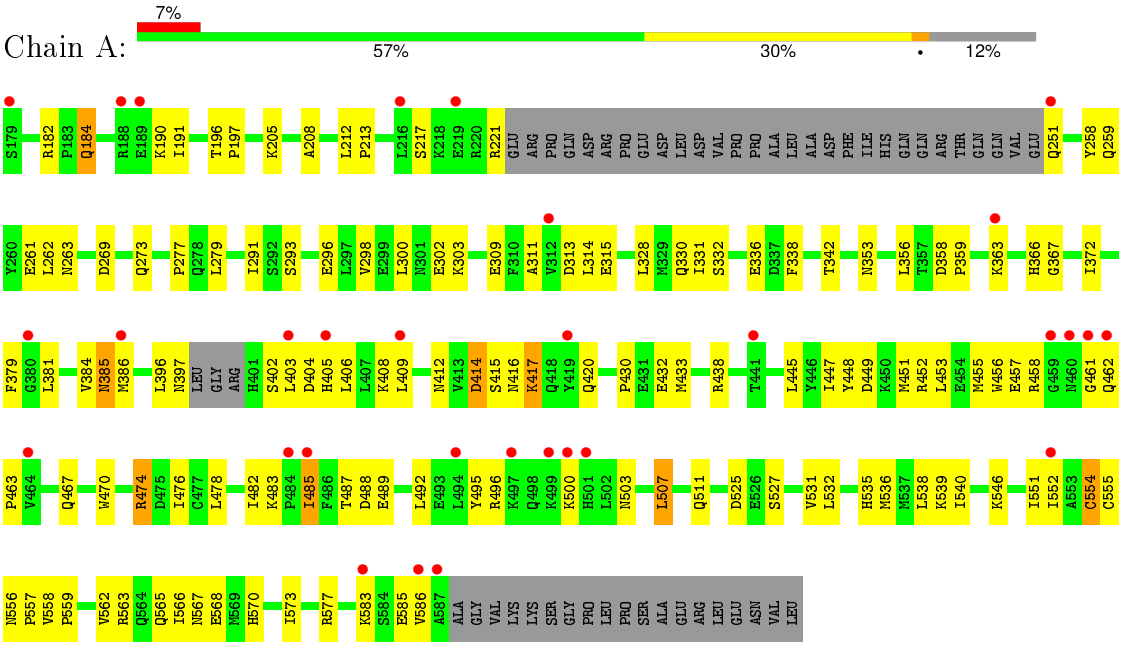
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	134	Total	O	0	0
			134	134		

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.

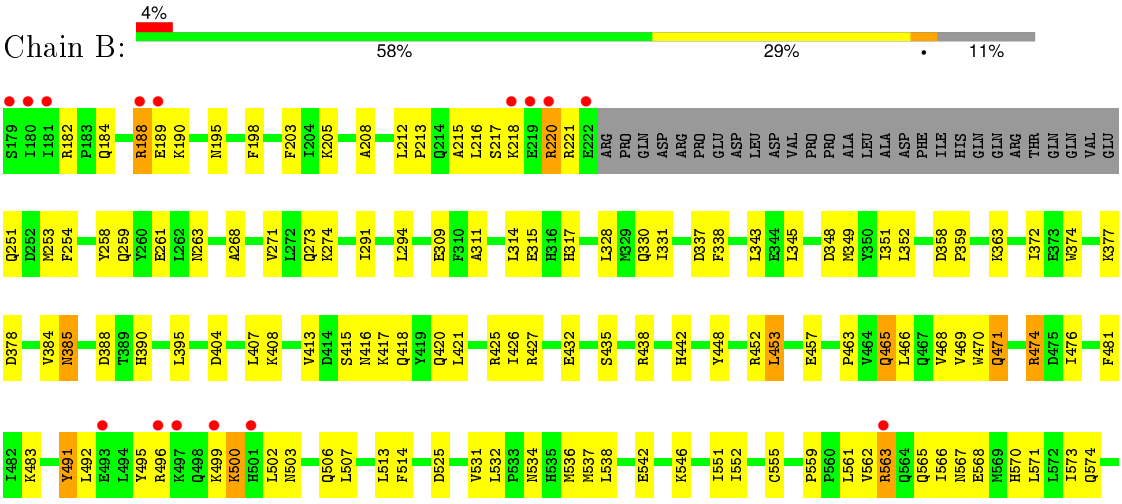
- Molecule 1: Exosome component 10

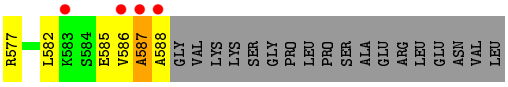
Chain A:



- Molecule 1: Exosome component 10

Chain B:




R577
L582
K583
S584
E585
V586
A587
A588
GLY
VAL
LYS
LYS
SER
GLY
PRO
LEU
PRO
SER
ALA
GLU
ARG
LEU
GLU
ASN
VAL
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	141.00Å 141.00Å 58.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.99 – 2.65 24.99 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.99-2.65) 99.6 (24.99-2.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.60 (at 2.64Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.215 , 0.265 0.213 , 0.266	Depositor DCC
R_{free} test set	1683 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.7	EDS
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 33644 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6506	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, YT3

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	0.38	0/3208	0.58	0/4343
1	B	0.39	0/3242	0.61	0/4390
All	All	0.38	0/6450	0.60	0/8733

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	3133	0	3123	116	0
1	B	3166	0	3158	94	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	B	2	0	0	0	0
4	A	68	0	0	4	0
4	B	134	0	0	4	0
All	All	6506	0	6281	210	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 17.

All (210) 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:586:VAL:HG23	1:B:587:ALA:H	1.29	0.96
1:A:536:MET:HE3	1:A:555:CYS:HB3	1.49	0.93
1:A:417:LYS:HE3	1:A:420:GLN:OE1	1.69	0.90
1:A:366:HIS:CE1	1:A:402:SER:HB3	2.08	0.89
1:B:188:ARG:NE	1:B:188:ARG:HA	1.91	0.86
1:A:258:TYR:HD1	1:A:261:GLU:HG3	1.43	0.83
1:A:293:SER:OG	1:A:296:GLU:HG2	1.79	0.82
1:A:366:HIS:HE1	1:A:402:SER:HB3	1.47	0.80
1:B:536:MET:HE3	1:B:555:CYS:HB3	1.63	0.79
1:A:291:ILE:HG23	1:A:296:GLU:HB2	1.63	0.79
1:A:552:ILE:HD13	1:A:563:ARG:CZ	2.16	0.76
1:A:495:TYR:O	1:A:500:LYS:HB2	1.86	0.74
1:A:462:GLN:NE2	1:A:463:PRO:HD2	2.02	0.74
1:A:488:ASP:OD2	1:A:511:GLN:HG2	1.88	0.74
1:A:403:LEU:HA	1:A:406:LEU:HB2	1.71	0.73
1:B:188:ARG:HE	1:B:188:ARG:HA	1.54	0.71
1:B:586:VAL:HG23	1:B:587:ALA:N	2.05	0.70
1:B:463:PRO:HG2	1:B:466:LEU:HD22	1.74	0.68
1:B:552:ILE:HD13	1:B:563:ARG:NH2	2.09	0.68
1:A:552:ILE:HG23	1:A:558:VAL:HG21	1.77	0.67
1:B:205:LYS:HG2	1:B:208:ALA:HB2	1.76	0.67
1:A:539:LYS:HG3	1:A:554:CYS:SG	2.34	0.66
1:A:474:ARG:HH11	1:A:474:ARG:HG2	1.60	0.66
1:B:317:HIS:CD2	1:B:425:ARG:HD3	2.31	0.66
1:B:492:LEU:O	1:B:496:ARG:HB2	1.95	0.66
1:A:191:ILE:HD12	1:A:191:ILE:H	1.61	0.66
1:A:191:ILE:HD12	1:A:191:ILE:N	2.11	0.65
1:B:315:GLU:HA	1:B:315:GLU:OE1	1.98	0.64
1:A:453:LEU:O	1:A:457:GLU:HG3	1.98	0.63
1:A:540:ILE:HD13	1:A:551:ILE:HG23	1.81	0.63
1:B:217:SER:HB3	1:B:220:ARG:HB2	1.80	0.62
1:A:396:LEU:HA	1:A:458:ARG:HH12	1.64	0.62
1:A:503:ASN:HB2	1:A:585:GLU:OE1	2.00	0.62
1:B:586:VAL:CG2	1:B:587:ALA:H	2.10	0.62
1:A:496:ARG:HH21	1:A:500:LYS:HE3	1.64	0.61
1:A:495:TYR:CE1	1:A:538:LEU:HD22	2.35	0.61
1:B:586:VAL:C	1:B:588:ALA:H	2.02	0.61
1:B:351:ILE:HG13	1:B:352:LEU:N	2.15	0.61
1:B:198:PHE:HB2	1:B:483:LYS:HG2	1.81	0.61
1:A:402:SER:HB2	4:A:164:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASP:O	1:A:273:GLN:HG3	2.00	0.61
1:A:196:THR:O	1:A:483:LYS:HD2	2.00	0.60
1:A:559:PRO:HG2	1:A:562:VAL:CG2	2.32	0.60
1:A:463:PRO:O	1:A:467:GLN:HG3	2.02	0.60
1:B:448:TYR:CE1	1:B:452:ARG:HD2	2.36	0.60
1:A:205:LYS:HG2	1:A:208:ALA:HB2	1.84	0.60
1:A:462:GLN:HE21	1:A:463:PRO:HD2	1.67	0.59
1:A:315:GLU:HB2	1:A:328:LEU:HB3	1.84	0.59
1:A:291:ILE:HG23	1:A:296:GLU:CB	2.29	0.59
1:B:496:ARG:O	1:B:499:LYS:HD2	2.04	0.58
1:B:216:LEU:HA	1:B:221:ARG:HH21	1.68	0.58
1:B:552:ILE:HD13	1:B:563:ARG:HH21	1.68	0.58
1:B:416:ASN:HB3	4:B:76:HOH:O	2.03	0.58
1:A:217:SER:O	1:A:221:ARG:HG3	2.04	0.57
1:A:492:LEU:HD22	1:A:507:LEU:HD11	1.86	0.57
1:A:448:TYR:O	1:A:452:ARG:HD3	2.04	0.57
1:A:448:TYR:CE1	1:A:452:ARG:HD2	2.40	0.57
1:B:190:LYS:HA	4:B:75:HOH:O	2.04	0.56
1:B:491:TYR:HE2	1:B:534:ASN:ND2	2.03	0.56
1:A:568:GLU:HB2	4:A:176:HOH:O	2.06	0.56
1:A:438:ARG:HD3	4:A:42:HOH:O	2.05	0.56
1:B:559:PRO:HG2	1:B:562:VAL:CG2	2.36	0.56
1:B:343:LEU:HD12	1:B:427:ARG:HH12	1.72	0.55
1:A:546:LYS:HG3	1:A:577:ARG:NH1	2.21	0.55
1:A:313:ASP:O	1:A:314:LEU:HD12	2.06	0.55
1:A:485:ILE:O	1:A:485:ILE:HD12	2.06	0.55
1:A:353:ASN:HB2	4:A:93:HOH:O	2.07	0.54
1:B:491:TYR:N	1:B:491:TYR:CD1	2.75	0.54
1:B:212:LEU:HD12	1:B:213:PRO:HD2	1.88	0.54
1:A:474:ARG:CG	1:A:474:ARG:HH11	2.20	0.54
1:B:216:LEU:CA	1:B:221:ARG:HH21	2.21	0.54
1:B:182:ARG:NH2	1:B:525:ASP:O	2.41	0.54
1:A:313:ASP:C	1:A:314:LEU:HD12	2.29	0.54
1:B:395:LEU:HD11	1:B:468:VAL:HG12	1.89	0.54
1:A:261:GLU:CD	1:A:261:GLU:H	2.12	0.53
1:B:465:GLN:O	1:B:469:VAL:HG23	2.08	0.53
1:B:253:MET:HG3	1:B:254:PHE:CD1	2.43	0.53
1:B:582:LEU:HB2	1:B:585:GLU:HG3	1.89	0.53
1:B:311:ALA:O	1:B:331:ILE:HA	2.09	0.53
1:A:182:ARG:NH2	1:A:525:ASP:O	2.42	0.53
1:A:405:HIS:NE2	1:A:409:LEU:HD22	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:GLN:NE2	1:B:568:GLU:OE1	2.42	0.52
1:B:317:HIS:HB2	4:B:11:HOH:O	2.09	0.52
1:A:546:LYS:HG3	1:A:577:ARG:HH12	1.75	0.52
1:B:258:TYR:HD1	1:B:261:GLU:HG3	1.75	0.52
1:B:570:HIS:NE2	1:B:574:GLN:OE1	2.43	0.52
1:B:294:LEU:HD13	1:B:348:ASP:HB3	1.92	0.52
1:B:345:LEU:O	1:B:349:MET:HG2	2.10	0.52
1:A:396:LEU:HA	1:A:458:ARG:NH1	2.25	0.52
1:A:546:LYS:HD2	1:A:577:ARG:HH22	1.75	0.52
1:A:482:ILE:HD12	1:A:482:ILE:N	2.25	0.52
1:A:303:LYS:NZ	1:A:336:GLU:OE2	2.41	0.51
1:B:404:ASP:OD1	1:B:408:LYS:HE3	2.11	0.51
1:A:552:ILE:HG13	1:A:566:ILE:HD13	1.92	0.51
1:B:259:GLN:HE21	1:B:263:ASN:HD21	1.57	0.51
1:A:451:MET:O	1:A:455:MET:HB2	2.11	0.51
1:A:291:ILE:CD1	1:A:300:LEU:HD22	2.41	0.51
1:A:356:LEU:HD12	1:A:381:LEU:HD22	1.93	0.51
1:A:262:LEU:O	1:A:474:ARG:HD3	2.11	0.50
1:A:536:MET:CE	1:A:555:CYS:HB3	2.31	0.50
1:A:566:ILE:HG23	1:A:567:ASN:N	2.26	0.50
1:A:384:VAL:O	1:A:385:ASN:HB3	2.10	0.50
1:A:583:LYS:O	1:A:586:VAL:HG22	2.11	0.50
1:A:300:LEU:HD13	1:A:338:PHE:CD2	2.46	0.50
1:B:213:PRO:HB3	1:B:251:GLN:HB3	1.94	0.50
1:B:420:GLN:O	1:B:421:LEU:HD23	2.13	0.49
1:B:377:LYS:HE2	1:B:481:PHE:CZ	2.47	0.49
1:B:465:GLN:H	1:B:465:GLN:CD	2.14	0.49
1:A:408:LYS:HE3	1:A:414:ASP:HB3	1.95	0.49
1:A:366:HIS:CE1	1:A:403:LEU:H	2.31	0.48
1:A:445:LEU:O	1:A:448:TYR:HB3	2.13	0.48
1:B:315:GLU:HB2	1:B:328:LEU:HB3	1.96	0.48
1:A:182:ARG:HB3	1:A:184:GLN:NE2	2.28	0.48
1:A:298:VAL:O	1:A:302:GLU:HG2	2.14	0.48
1:B:217:SER:O	1:B:221:ARG:HG2	2.14	0.48
1:A:366:HIS:CD2	1:A:403:LEU:HB2	2.49	0.48
1:B:448:TYR:CD1	1:B:452:ARG:HD2	2.50	0.47
1:A:430:PRO:HG2	1:A:433:MET:HG3	1.97	0.47
1:B:216:LEU:HD22	1:B:221:ARG:HH22	1.80	0.47
1:B:551:ILE:HD11	1:B:570:HIS:HA	1.97	0.47
1:A:212:LEU:HD12	1:A:213:PRO:HD2	1.97	0.47
1:B:471:GLN:O	1:B:474:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ALA:O	1:A:331:ILE:HA	2.15	0.47
1:A:402:SER:O	1:A:405:HIS:N	2.48	0.47
1:A:453:LEU:C	1:A:455:MET:H	2.17	0.47
1:A:363:LYS:HE2	1:A:385:ASN:O	2.15	0.47
1:A:258:TYR:CD1	1:A:261:GLU:HG3	2.34	0.47
1:B:363:LYS:HE2	1:B:385:ASN:O	2.15	0.47
1:A:196:THR:CG2	1:A:197:PRO:HD2	2.45	0.46
1:B:337:ASP:OD2	1:B:442:HIS:ND1	2.43	0.46
1:A:536:MET:HE3	1:A:559:PRO:HD3	1.98	0.46
1:B:377:LYS:HB2	1:B:481:PHE:CD2	2.50	0.46
1:A:496:ARG:HA	1:A:500:LYS:HB2	1.97	0.46
1:B:343:LEU:HD12	1:B:427:ARG:NH1	2.30	0.46
1:B:538:LEU:O	1:B:542:GLU:HG3	2.16	0.46
1:A:372:ILE:HG13	1:A:476:ILE:HG22	1.98	0.46
1:B:546:LYS:HE2	1:B:577:ARG:NH2	2.31	0.46
1:B:404:ASP:O	1:B:408:LYS:HG3	2.16	0.46
1:A:573:ILE:O	1:A:577:ARG:HG3	2.16	0.45
1:A:474:ARG:CG	1:A:474:ARG:NH1	2.77	0.45
1:B:216:LEU:HD22	1:B:221:ARG:NH2	2.31	0.45
1:A:184:GLN:H	1:A:184:GLN:HE21	1.65	0.45
1:B:432:GLU:H	1:B:432:GLU:CD	2.20	0.45
1:A:496:ARG:CZ	1:A:496:ARG:HB2	2.45	0.45
1:A:396:LEU:O	1:A:397:ASN:HB2	2.16	0.45
1:A:213:PRO:HB3	1:A:251:GLN:HB3	1.97	0.45
1:B:291:ILE:HD11	1:B:338:PHE:HD2	1.82	0.45
1:A:503:ASN:HB2	1:A:585:GLU:CD	2.38	0.44
1:A:535:HIS:NE2	1:A:536:MET:HG3	2.32	0.44
1:B:418:GLN:HG2	1:B:418:GLN:O	2.17	0.44
1:A:565:GLN:HE21	1:A:565:GLN:HA	1.83	0.44
1:B:374:TRP:O	1:B:378:ASP:HB2	2.17	0.44
1:A:300:LEU:HD13	1:A:338:PHE:CE2	2.52	0.44
1:A:184:GLN:H	1:A:184:GLN:NE2	2.15	0.44
1:A:559:PRO:HG2	1:A:562:VAL:HB	2.00	0.44
1:B:395:LEU:HD12	1:B:469:VAL:HG22	1.98	0.44
1:B:502:LEU:HA	1:B:506:GLN:OE1	2.17	0.44
1:A:500:LYS:NZ	1:A:500:LYS:HB3	2.33	0.44
1:B:215:ALA:HA	1:B:220:ARG:HG2	2.00	0.44
1:A:262:LEU:HB2	1:A:478:LEU:HD21	1.99	0.44
1:A:363:LYS:HD3	1:A:363:LYS:N	2.33	0.44
1:A:363:LYS:O	1:A:386:MET:HG2	2.18	0.44
1:A:551:ILE:O	1:A:554:CYS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:PHE:HD1	1:B:218:LYS:HG2	1.82	0.43
1:B:388:ASP:OD1	1:B:390:HIS:HB3	2.19	0.43
1:A:205:LYS:O	1:A:208:ALA:HB2	2.19	0.43
1:B:268:ALA:O	1:B:271:VAL:HG22	2.18	0.43
1:B:551:ILE:HB	1:B:566:ILE:HD11	1.99	0.43
1:B:435:SER:O	1:B:438:ARG:HG2	2.19	0.43
1:B:502:LEU:HB2	1:B:507:LEU:CD1	2.49	0.43
1:A:432:GLU:OE2	1:A:432:GLU:N	2.47	0.43
1:B:571:LEU:HB3	4:B:149:HOH:O	2.19	0.43
1:B:261:GLU:CD	1:B:261:GLU:H	2.21	0.42
1:B:384:VAL:O	1:B:385:ASN:HB3	2.19	0.42
1:A:358:ASP:HA	1:A:359:PRO:HD2	1.88	0.42
1:A:551:ILE:HD11	1:A:570:HIS:HA	2.00	0.42
1:B:531:VAL:HG22	1:B:561:LEU:HD12	2.01	0.42
1:B:491:TYR:HD1	1:B:491:TYR:H	1.66	0.42
1:B:273:GLN:O	1:B:274:LYS:C	2.58	0.42
1:B:536:MET:HE2	1:B:536:MET:HB3	1.83	0.42
1:A:565:GLN:NE2	1:A:565:GLN:HA	2.34	0.42
1:B:513:LEU:HD21	1:B:573:ILE:HD11	2.02	0.42
1:A:277:PRO:HA	1:A:449:ASP:HB3	2.02	0.41
1:B:453:LEU:O	1:B:457:GLU:HG3	2.20	0.41
1:B:495:TYR:HB3	1:B:500:LYS:HB2	2.01	0.41
1:B:372:ILE:HG13	1:B:476:ILE:HG22	2.01	0.41
1:B:503:ASN:OD1	1:B:506:GLN:HG3	2.20	0.41
1:A:485:ILE:H	1:A:485:ILE:HD12	1.85	0.41
1:A:495:TYR:C	1:A:500:LYS:HB2	2.40	0.41
1:A:311:ALA:HB3	1:A:332:SER:HB2	2.03	0.41
1:B:407:LEU:CD1	1:B:415:SER:HB3	2.50	0.41
1:A:447:ILE:O	1:A:451:MET:HG3	2.21	0.41
1:B:358:ASP:C	1:B:358:ASP:OD2	2.59	0.41
1:B:358:ASP:HA	1:B:359:PRO:HD2	1.89	0.41
1:B:408:LYS:HG2	1:B:413:VAL:O	2.20	0.41
1:A:556:ASN:HA	1:A:557:PRO:HA	1.88	0.41
1:A:291:ILE:HD12	1:A:300:LEU:HD22	2.01	0.41
1:B:417:LYS:HE2	1:B:420:GLN:HG2	2.03	0.41
1:B:426:ILE:O	1:B:426:ILE:HG23	2.21	0.41
1:A:496:ARG:NH2	1:A:500:LYS:HE3	2.35	0.41
1:A:259:GLN:O	1:A:263:ASN:ND2	2.54	0.41
1:A:527:SER:O	1:A:531:VAL:HG23	2.21	0.41
1:A:190:LYS:HG3	1:A:191:ILE:N	2.36	0.40
1:B:566:ILE:HG23	1:B:567:ASN:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:ILE:O	1:B:577:ARG:HG3	2.21	0.40
1:A:456:TRP:CE2	1:A:461:GLY:HA2	2.57	0.40
1:A:487:THR:HB	1:A:489:GLU:OE1	2.21	0.40
1:A:402:SER:HB3	1:A:403:LEU:H	1.69	0.40
1:A:342:THR:HB	1:A:379:PHE:CZ	2.57	0.40
1:B:514:PHE:HA	1:B:537:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	371/428 (87%)	338 (91%)	27 (7%)	6 (2%)	12 26
1	B	378/428 (88%)	358 (95%)	18 (5%)	2 (0%)	34 59
All	All	749/856 (88%)	696 (93%)	45 (6%)	8 (1%)	17 38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	417	LYS
1	A	385	ASN
1	B	587	ALA
1	A	416	ASN
1	A	554	CYS
1	B	385	ASN
1	A	415	SER
1	A	367	GLY

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	350/394 (89%)	338 (97%)	12 (3%)	44 72
1	B	352/394 (89%)	335 (95%)	17 (5%)	31 59
All	All	702/788 (89%)	673 (96%)	29 (4%)	37 66

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	279	LEU
1	A	309	GLU
1	A	330	GLN
1	A	404	ASP
1	A	412	ASN
1	A	414	ASP
1	A	470	TRP
1	A	474	ARG
1	A	485	ILE
1	A	507	LEU
1	A	532	LEU
1	B	184	GLN
1	B	188	ARG
1	B	189	GLU
1	B	195	ASN
1	B	220	ARG
1	B	309	GLU
1	B	314	LEU
1	B	330	GLN
1	B	453	LEU
1	B	465	GLN
1	B	470	TRP
1	B	471	GLN
1	B	474	ARG
1	B	491	TYR
1	B	500	LYS

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Mol	Chain	Res	Type
1	B	532	LEU
1	B	563	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	263	ASN
1	A	278	GLN
1	A	316	HIS
1	A	330	GLN
1	A	412	ASN
1	A	462	GLN
1	A	498	GLN
1	A	505	GLN
1	A	511	GLN
1	A	564	GLN
1	A	565	GLN
1	A	570	HIS
1	B	263	ASN
1	B	278	GLN
1	B	498	GLN
1	B	505	GLN
1	B	565	GLN

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

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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

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	377/428 (88%)	0.44	31 (8%)	14	11	46, 74, 105, 120	0
1	B	382/428 (89%)	0.16	19 (4%)	32	30	37, 58, 96, 116	0
All	All	759/856 (88%)	0.30	50 (6%)	22	19	37, 66, 104, 120	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	587	ALA	7.6
1	A	587	ALA	6.4
1	B	222	GLU	5.5
1	B	588	ALA	5.0
1	B	179	SER	4.8
1	A	405	HIS	4.4
1	A	462	GLN	4.0
1	B	181	ILE	4.0
1	A	188	ARG	3.8
1	B	496	ARG	3.8
1	A	459	GLY	3.7
1	B	180	ILE	3.7
1	A	461	GLY	3.7
1	A	497	LYS	3.7
1	B	497	LYS	3.6
1	A	179	SER	3.4
1	B	188	ARG	3.3
1	A	251	GLN	3.2
1	A	460	ASN	3.2
1	A	586	VAL	3.2
1	B	493	GLU	3.2
1	A	464	VAL	3.2
1	B	586	VAL	3.1
1	B	220	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	499	LYS	2.9
1	A	552	ILE	2.8
1	A	363	LYS	2.8
1	B	583	LYS	2.8
1	A	403	LEU	2.7
1	A	501	HIS	2.7
1	A	441	THR	2.6
1	A	216	LEU	2.6
1	B	501	HIS	2.5
1	B	189	GLU	2.5
1	B	218	LYS	2.5
1	B	219	GLU	2.5
1	A	312	VAL	2.4
1	A	500	LYS	2.3
1	A	386	MET	2.3
1	A	380	GLY	2.3
1	A	499	LYS	2.2
1	A	409	LEU	2.2
1	A	494	LEU	2.2
1	A	189	GLU	2.2
1	A	583	LYS	2.1
1	A	484	PRO	2.1
1	A	419	TYR	2.1
1	B	563	ARG	2.1
1	A	219	GLU	2.1
1	A	485	ILE	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	MG	B	2	1/1	0.88	0.36	11.28	62,62,62,62	0
2	YT3	A	3	1/1	0.99	0.19	-0.50	75,75,75,75	0
2	YT3	A	1	1/1	0.91	0.13	-1.02	100,100,100,100	0
2	YT3	B	607	1/1	0.99	0.13	-	59,59,59,59	0
3	MG	B	1	1/1	0.73	0.22	-	74,74,74,74	0

6.5 Other polymers (i)

There are no such residues in this entry.