Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 09:46 AM EDT

PDB ID	:	3SAG
Title	:	Crystal structure of the human RRP6 catalytic domain with D313N mutation in the active site
Authors	:	Januszyk, K.; Liu, Q.; Lima, C.D.
Deposited on	:	2011-06-02
Resolution	:	2.70 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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)	:	2.35

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 2.70 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	Percentile Ranks	Value
Rfree		0.257
Clashscore		14
Ramachandran outliers		0.4%
Sidechain outliers		4.7%
RSRZ outliers		4.3%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
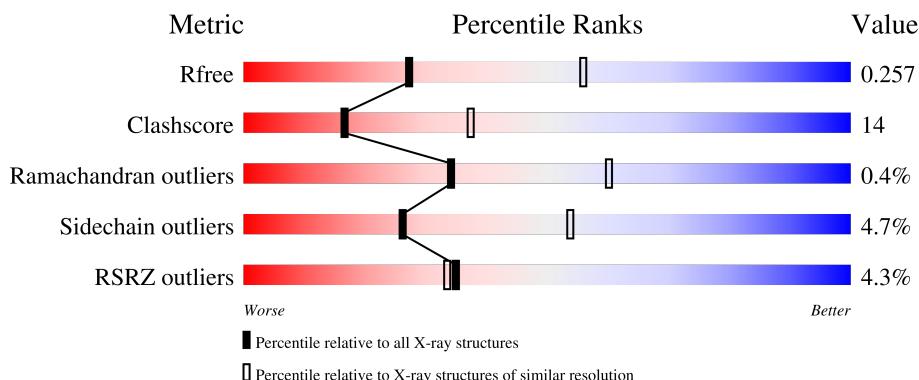
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	428	4% / 60% / 28% / • / 11%
1	B	428	4% / 62% / 25% / • / 11%
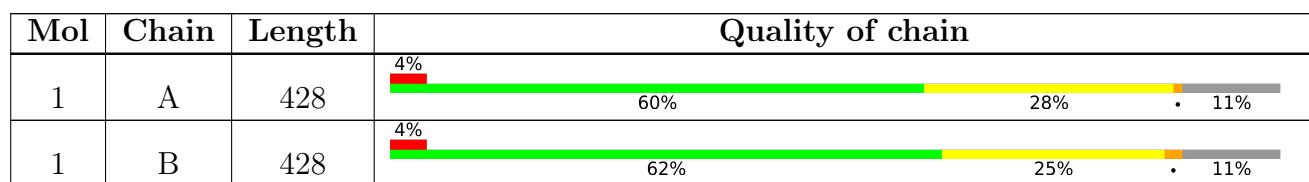
2   Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6537 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	381	Total 3168	C 2029	N 548	O 573	S 18	0	0	0
1	B	380	Total 3137	C 2010	N 537	O 572	S 18	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	SER	-	expression tag	UNP Q01780
A	313	ASN	ASP	engineered mutation	UNP Q01780
B	179	SER	-	expression tag	UNP Q01780
B	313	ASN	ASP	engineered mutation	UNP Q01780

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total 114	O 114	0	0

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	114	Total 114	O 114	0	0

3 Residue-property plots ⓘ

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: Exosome component 10

Chain A:

• Molecule 1: Exosome component 10

Chain B:
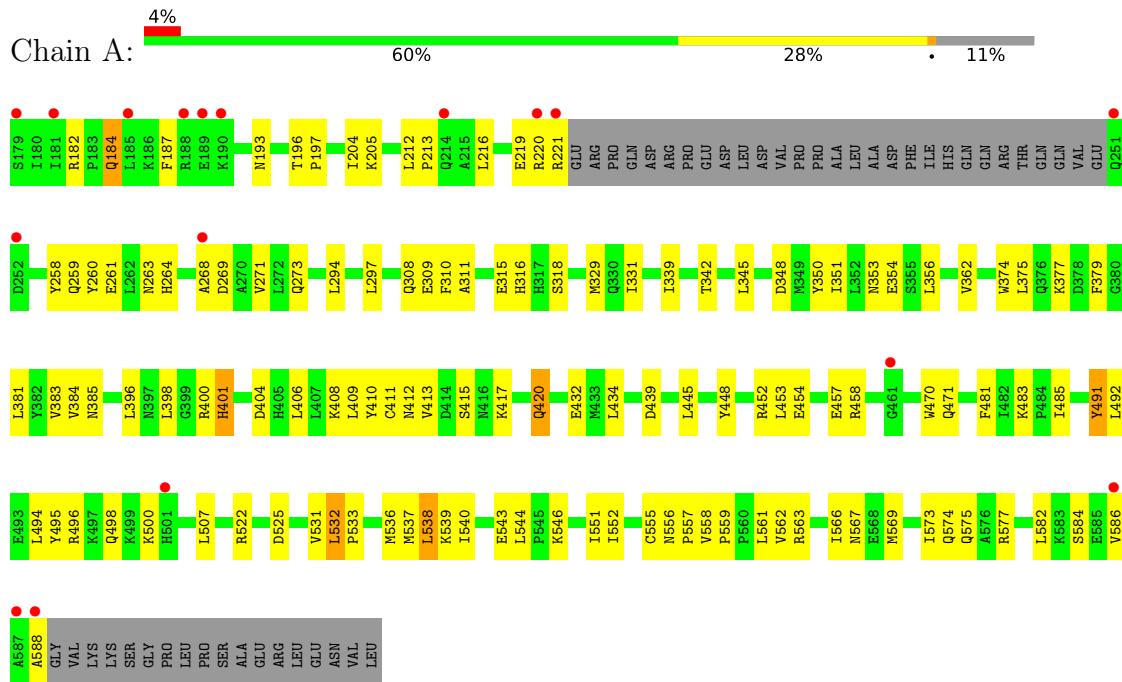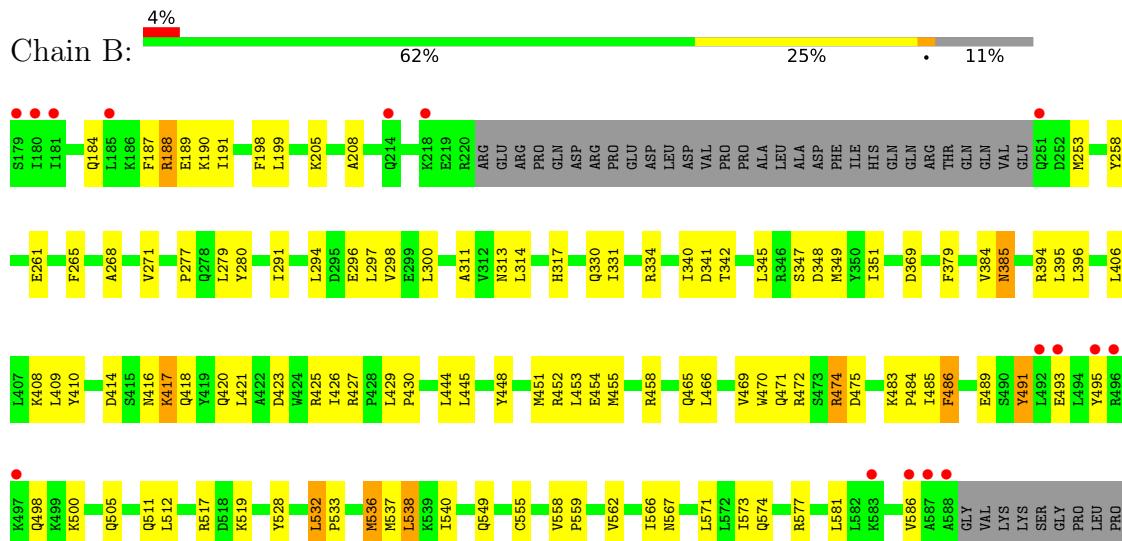
SER ALA GLU ARG LEU GLU ASN VAL LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	138.80Å 138.80Å 60.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.70 – 2.70 34.70 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.70-2.70) 99.8 (34.70-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.42 (at 2.68Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.208 , 0.262 0.203 , 0.257	Depositor DCC
R_{free} test set	1590 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.1	EDS
L-test for twinning [2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6537	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

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

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	0.36	0/3245	0.58	0/4394
1	B	0.38	0/3213	0.59	0/4355
All	All	0.37	0/6458	0.58	0/8749

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	3168	0	3162	88	0
1	B	3137	0	3110	90	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	B	1	0	0	0	0
4	A	114	0	0	4	0
4	B	114	0	0	2	0
All	All	6537	0	6272	178	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 14.

All (178) 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:416:ASN:HB2	1:B:418:GLN:HE21	1.36	0.88
1:B:394:ARG:HH22	1:B:472:ARG:HE	1.18	0.88
1:B:571:LEU:HA	1:B:574:GLN:HE21	1.43	0.83
1:A:494:LEU:HG	1:A:498:GLN:HE21	1.44	0.81
1:B:394:ARG:NH2	1:B:472:ARG:HE	1.82	0.78
1:B:396:LEU:HD21	1:B:455:MET:HG2	1.66	0.78
1:A:258:TYR:HD1	1:A:261:GLU:HG3	1.50	0.76
1:B:416:ASN:HB2	1:B:418:GLN:NE2	2.02	0.74
1:A:362:VAL:HG22	1:A:385:ASN:HD21	1.52	0.74
1:B:297:LEU:HD22	1:B:345:LEU:HD13	1.70	0.73
1:A:485:ILE:O	1:A:485:ILE:HD12	1.88	0.73
1:B:258:TYR:HD1	1:B:261:GLU:HG3	1.53	0.73
1:A:294:LEU:HD13	1:A:348:ASP:HB3	1.71	0.72
1:B:205:LYS:HG2	1:B:208:ALA:HB2	1.72	0.71
1:A:533:PRO:HG2	1:A:536:MET:HG3	1.72	0.71
1:B:505:GLN:HE21	1:B:581:LEU:HG	1.57	0.69
1:A:556:ASN:HA	4:A:127:HOH:O	1.93	0.68
1:B:417:LYS:HD2	1:B:417:LYS:H	1.58	0.68
1:A:552:ILE:HG23	1:A:558:VAL:HG21	1.75	0.68
1:A:182:ARG:NH1	1:A:182:ARG:HB3	2.10	0.67
1:A:362:VAL:CG2	1:A:385:ASN:HD21	2.07	0.67
1:B:491:TYR:H	1:B:491:TYR:HD1	1.45	0.64
1:B:191:ILE:HD12	1:B:191:ILE:N	2.12	0.64
1:A:538:LEU:HD22	1:A:538:LEU:O	1.97	0.64
1:B:187:PHE:HD2	1:B:191:ILE:HD11	1.62	0.63
1:A:259:GLN:HE21	1:A:263:ASN:HD21	1.45	0.63
1:A:448:TYR:CE1	1:A:452:ARG:HD2	2.34	0.62
1:A:269:ASP:O	1:A:273:GLN:HG3	2.00	0.61
1:A:532:LEU:HD13	1:A:537:MET:HB2	1.81	0.61
1:A:184:GLN:HA	1:A:187:PHE:CD2	2.37	0.59
1:B:296:GLU:HA	1:B:296:GLU:OE1	2.01	0.59
1:B:294:LEU:HD13	1:B:348:ASP:HB3	1.85	0.59
1:A:213:PRO:HG2	1:A:216:LEU:HD12	1.83	0.59
1:B:573:ILE:O	1:B:577:ARG:HG3	2.02	0.59
1:A:362:VAL:HG22	1:A:385:ASN:ND2	2.16	0.59
1:B:495:TYR:HB3	1:B:500:LYS:CB	2.33	0.59
1:B:279:LEU:HD13	1:B:280:TYR:O	2.03	0.59
1:B:340:ILE:HG23	1:B:345:LEU:HD12	1.85	0.58
1:A:353:ASN:ND2	1:A:381:LEU:HD23	2.19	0.58
1:A:557:PRO:HA	4:A:127:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:C	1:A:400:ARG:H	2.07	0.57
1:B:559:PRO:HG2	1:B:562:VAL:CG2	2.34	0.57
1:A:552:ILE:HD13	1:A:563:ARG:NH2	2.21	0.56
1:B:294:LEU:O	1:B:298:VAL:HG23	2.06	0.56
1:A:533:PRO:HD2	1:A:536:MET:HE2	1.88	0.56
1:A:182:ARG:HB3	1:A:182:ARG:HH11	1.70	0.56
1:B:532:LEU:HD21	1:B:536:MET:HB3	1.88	0.56
1:A:184:GLN:HE21	1:A:184:GLN:H	1.53	0.55
1:A:268:ALA:O	1:A:271:VAL:HG22	2.06	0.55
1:B:474:ARG:HD2	1:B:474:ARG:C	2.27	0.55
1:B:394:ARG:HH22	1:B:472:ARG:NE	1.96	0.55
1:A:351:ILE:O	1:A:354:GLU:HG3	2.06	0.54
1:A:495:TYR:O	1:A:500:LYS:HB2	2.07	0.54
1:A:491:TYR:H	1:A:491:TYR:HD1	1.55	0.54
1:B:258:TYR:CD1	1:B:261:GLU:HG3	2.39	0.54
1:A:453:LEU:O	1:A:457:GLU:HG3	2.08	0.54
1:A:398:LEU:C	1:A:400:ARG:N	2.61	0.53
1:B:420:GLN:O	1:B:421:LEU:HB2	2.07	0.53
1:A:398:LEU:HD22	1:A:401:HIS:NE2	2.24	0.53
1:B:188:ARG:HG3	1:B:347:SER:HB3	1.91	0.53
1:B:559:PRO:HG2	1:B:562:VAL:HB	1.91	0.53
1:A:409:LEU:HD12	1:A:409:LEU:O	2.09	0.52
1:A:540:ILE:HD13	1:A:551:ILE:HG23	1.91	0.52
1:A:212:LEU:HD12	1:A:213:PRO:HD2	1.92	0.52
1:A:311:ALA:O	1:A:331:ILE:HA	2.09	0.52
1:B:533:PRO:HD2	1:B:536:MET:HE2	1.91	0.52
1:B:472:ARG:O	1:B:475:ASP:HB2	2.10	0.52
1:B:505:GLN:HE21	1:B:581:LEU:CG	2.22	0.52
1:B:317:HIS:CD2	1:B:425:ARG:HD3	2.45	0.52
1:B:445:LEU:O	1:B:448:TYR:HB3	2.10	0.51
1:B:484:PRO:HB2	1:B:486:PHE:CZ	2.45	0.51
1:A:182:ARG:HH11	1:A:182:ARG:CB	2.23	0.51
1:B:455:MET:SD	1:B:466:LEU:HD12	2.51	0.51
1:B:489:GLU:O	1:B:493:GLU:HG3	2.10	0.51
1:B:517:ARG:NE	1:B:528:TYR:HD2	2.08	0.51
1:B:369:ASP:HB2	4:B:162:HOH:O	2.10	0.51
1:A:494:LEU:HG	1:A:498:GLN:NE2	2.21	0.50
1:A:193:ASN:O	1:A:522:ARG:HD3	2.11	0.50
1:B:491:TYR:CD1	1:B:491:TYR:N	2.75	0.50
1:A:555:CYS:HB2	1:A:558:VAL:HG22	1.93	0.50
1:B:536:MET:HE3	1:B:559:PRO:CD	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:LEU:CD2	1:B:536:MET:HB3	2.41	0.50
1:B:536:MET:CE	1:B:559:PRO:HD3	2.41	0.50
1:B:495:TYR:HA	1:B:498:GLN:HB3	1.93	0.50
1:A:260:TYR:CE1	1:A:264:HIS:CE1	3.00	0.49
1:A:377:LYS:HG3	1:A:481:PHE:CE2	2.48	0.49
1:A:182:ARG:NH2	1:A:525:ASP:O	2.46	0.49
1:A:310:PHE:HD1	1:A:331:ILE:HG23	1.77	0.49
1:B:454:GLU:O	1:B:458:ARG:HG2	2.12	0.49
1:B:265:PHE:CZ	1:B:385:ASN:HA	2.48	0.48
1:B:191:ILE:N	1:B:191:ILE:CD1	2.76	0.48
1:A:339:ILE:HD12	1:A:434:LEU:HD22	1.95	0.48
1:A:398:LEU:O	1:A:400:ARG:N	2.46	0.48
1:B:485:ILE:O	1:B:485:ILE:HG23	2.14	0.48
1:B:511:GLN:HG3	1:B:512:LEU:N	2.28	0.48
1:A:259:GLN:HE21	1:A:263:ASN:ND2	2.11	0.47
1:B:395:LEU:HD12	1:B:469:VAL:HG22	1.96	0.47
1:A:362:VAL:HA	1:A:385:ASN:ND2	2.29	0.47
1:A:408:LYS:HE2	1:A:412:ASN:OD1	2.15	0.47
1:A:445:LEU:O	1:A:448:TYR:HB3	2.14	0.47
1:B:555:CYS:HB2	1:B:558:VAL:HG22	1.95	0.47
1:B:448:TYR:CE1	1:B:452:ARG:HD2	2.49	0.47
1:A:491:TYR:N	1:A:491:TYR:CD1	2.82	0.47
1:B:190:LYS:HG2	1:B:191:ILE:N	2.29	0.47
1:B:313:ASN:C	1:B:314:LEU:HD12	2.35	0.47
1:B:409:LEU:HD12	1:B:409:LEU:O	2.13	0.47
1:A:582:LEU:O	1:A:586:VAL:HG23	2.15	0.47
1:A:559:PRO:HG2	1:A:562:VAL:CG2	2.44	0.47
1:B:349:MET:HB2	1:B:379:PHE:HB3	1.97	0.46
1:B:334:ARG:HD3	1:B:445:LEU:HD12	1.97	0.46
1:B:536:MET:O	1:B:540:ILE:HG13	2.15	0.46
1:A:411:CYS:HB2	1:A:413:VAL:HG23	1.98	0.46
1:A:404:ASP:OD1	1:A:415:SER:HB3	2.16	0.45
1:B:384:VAL:O	1:B:385:ASN:HB3	2.16	0.45
1:A:546:LYS:HG3	1:A:577:ARG:NH1	2.32	0.45
1:B:408:LYS:HE3	1:B:414:ASP:OD1	2.16	0.45
1:B:341:ASP:OD1	1:B:427:ARG:NH1	2.49	0.45
1:B:291:ILE:HD12	1:B:300:LEU:HD22	1.98	0.45
1:A:329:MET:HE3	1:A:375:LEU:HD21	1.98	0.45
1:A:353:ASN:HD21	1:A:381:LEU:HA	1.82	0.45
1:B:423:ASP:O	1:B:426:ILE:HG22	2.17	0.45
1:B:342:THR:HG22	1:B:349:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:HH12	1:A:184:GLN:HB2	1.82	0.44
1:A:384:VAL:O	1:A:385:ASN:HB3	2.17	0.44
1:B:187:PHE:CD2	1:B:191:ILE:HD11	2.49	0.44
1:B:536:MET:HE3	1:B:559:PRO:HD3	1.99	0.44
1:B:268:ALA:O	1:B:271:VAL:HG22	2.18	0.44
1:B:406:LEU:HD22	1:B:410:TYR:HE1	1.82	0.44
1:B:451:MET:O	1:B:455:MET:HG3	2.18	0.44
1:B:536:MET:HG2	1:B:555:CYS:SG	2.58	0.44
1:B:416:ASN:O	1:B:418:GLN:HG2	2.18	0.44
1:B:486:PHE:CD1	1:B:486:PHE:N	2.85	0.44
1:A:196:THR:O	1:A:483:LYS:HD2	2.18	0.43
1:B:505:GLN:NE2	1:B:581:LEU:HG	2.30	0.43
1:A:377:LYS:O	1:A:377:LYS:HG2	2.17	0.43
1:B:465:GLN:O	1:B:469:VAL:HG23	2.18	0.43
1:B:533:PRO:HD2	1:B:536:MET:CE	2.48	0.43
1:A:297:LEU:HD22	1:A:345:LEU:HD13	2.00	0.43
1:A:316:HIS:HB2	1:A:374:TRP:CZ3	2.53	0.43
1:A:350:TYR:CD1	1:A:351:ILE:N	2.87	0.43
1:A:406:LEU:O	1:A:410:TYR:HB2	2.18	0.43
1:A:342:THR:HB	1:A:379:PHE:CZ	2.54	0.43
1:A:492:LEU:O	1:A:496:ARG:HB2	2.18	0.43
1:A:562:VAL:HG13	1:A:569:MET:SD	2.59	0.43
1:A:445:LEU:HG	4:A:31:HOH:O	2.17	0.42
1:A:454:GLU:O	1:A:458:ARG:HG3	2.19	0.42
1:A:204:ILE:HG23	1:A:204:ILE:O	2.19	0.42
1:A:318:SER:HB2	4:A:172:HOH:O	2.18	0.42
1:B:199:LEU:HD13	1:B:253:MET:HE2	2.02	0.42
1:B:297:LEU:HG	1:B:351:ILE:HD11	2.01	0.42
1:B:423:ASP:OD1	1:B:425:ARG:HB2	2.19	0.42
1:B:311:ALA:O	1:B:331:ILE:HA	2.19	0.42
1:B:340:ILE:HD12	1:B:340:ILE:N	2.35	0.42
1:B:429:LEU:HA	1:B:430:PRO:HD2	1.91	0.42
1:A:584:SER:O	1:A:588:ALA:HB3	2.20	0.42
1:B:261:GLU:CD	1:B:261:GLU:H	2.23	0.42
1:B:566:ILE:HG23	1:B:567:ASN:N	2.35	0.42
1:A:566:ILE:HG23	1:A:567:ASN:N	2.35	0.42
1:B:538:LEU:O	1:B:538:LEU:HD23	2.19	0.42
1:B:559:PRO:HG2	1:B:562:VAL:CB	2.49	0.42
1:B:198:PHE:HB2	1:B:483:LYS:HG2	2.02	0.41
1:A:539:LYS:HE3	1:A:539:LYS:HB2	1.81	0.41
1:A:546:LYS:HG3	1:A:577:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:ILE:O	1:A:577:ARG:HG3	2.20	0.41
1:A:196:THR:HG23	1:A:197:PRO:HD2	2.01	0.41
1:A:531:VAL:HG22	1:A:561:LEU:CD1	2.51	0.41
1:B:341:ASP:CG	1:B:427:ARG:NH1	2.74	0.41
1:A:219:GLU:C	1:A:221:ARG:H	2.24	0.41
1:B:532:LEU:HD22	1:B:537:MET:HB2	2.03	0.41
1:A:205:LYS:HZ1	1:A:261:GLU:CD	2.24	0.40
1:A:258:TYR:CD1	1:A:261:GLU:HG3	2.41	0.40
1:B:536:MET:HE1	1:B:559:PRO:HD3	2.03	0.40
1:A:315:GLU:OE1	1:A:315:GLU:HA	2.21	0.40
1:A:417:LYS:HG2	1:A:420:GLN:HE22	1.85	0.40
1:A:543:GLU:O	1:A:544:LEU:C	2.60	0.40
1:A:356:LEU:O	1:A:383:VAL:HA	2.21	0.40
1:A:396:LEU:O	1:A:398:LEU:HG	2.21	0.40
1:B:334:ARG:HG2	4:B:19:HOH:O	2.22	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	377/428 (88%)	344 (91%)	32 (8%)	1 (0%)	41	66
1	B	376/428 (88%)	352 (94%)	22 (6%)	2 (0%)	29	54
All	All	753/856 (88%)	696 (92%)	54 (7%)	3 (0%)	34	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ARG
1	B	385	ASN
1	B	277	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	353/395 (89%)	338 (96%)	15 (4%)	30	58
1	B	348/395 (88%)	330 (95%)	18 (5%)	23	49
All	All	701/790 (89%)	668 (95%)	33 (5%)	26	54

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	308	GLN
1	A	309	GLU
1	A	401	HIS
1	A	420	GLN
1	A	432	GLU
1	A	439	ASP
1	A	470	TRP
1	A	471	GLN
1	A	491	TYR
1	A	507	LEU
1	A	532	LEU
1	A	538	LEU
1	A	574	GLN
1	A	575	GLN
1	B	184	GLN
1	B	188	ARG
1	B	189	GLU
1	B	330	GLN
1	B	417	LYS
1	B	444	LEU
1	B	453	LEU
1	B	470	TRP
1	B	471	GLN
1	B	474	ARG
1	B	486	PHE
1	B	491	TYR

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Mol	Chain	Res	Type
1	B	519	LYS
1	B	532	LEU
1	B	536	MET
1	B	538	LEU
1	B	549	GLN
1	B	586	VAL

Sometimes 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	259	GLN
1	A	385	ASN
1	A	465	GLN
1	A	467	GLN
1	A	471	GLN
1	A	498	GLN
1	A	505	GLN
1	A	575	GLN
1	B	184	GLN
1	B	259	GLN
1	B	278	GLN
1	B	313	ASN
1	B	418	GLN
1	B	420	GLN
1	B	462	GLN
1	B	505	GLN
1	B	574	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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, 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	381/428 (89%)	0.09	17 (4%)	33	31	42, 65, 97, 111	0
1	B	380/428 (88%)	0.06	16 (4%)	36	35	40, 61, 96, 125	0
All	All	761/856 (88%)	0.08	33 (4%)	35	33	40, 63, 97, 125	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	587	ALA	5.9
1	B	588	ALA	4.8
1	B	179	SER	4.6
1	B	496	ARG	4.6
1	A	588	ALA	4.4
1	B	181	ILE	3.8
1	A	586	VAL	3.7
1	A	587	ALA	3.6
1	A	189	GLU	3.5
1	B	218	LYS	3.5
1	A	179	SER	3.5
1	A	220	ARG	3.4
1	B	180	ILE	3.2
1	B	495	TYR	3.0
1	B	586	VAL	3.0
1	A	190	LYS	2.9
1	A	252	ASP	2.9
1	A	251	GLN	2.8
1	A	268	ALA	2.8
1	A	501	HIS	2.4
1	B	497	LYS	2.4
1	A	185	LEU	2.3
1	A	221	ARG	2.3
1	B	251	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	493	GLU	2.3
1	A	188	ARG	2.2
1	B	214	GLN	2.2
1	A	181	ILE	2.2
1	A	214	GLN	2.1
1	B	492	LEU	2.1
1	B	583	LYS	2.1
1	B	185	LEU	2.1
1	A	461	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
3	MG	B	1	1/1	0.90	0.27	60,60,60,60	0
2	YT3	A	1	1/1	0.98	0.09	63,63,63,63	0
2	YT3	A	3	1/1	0.99	0.11	71,71,71,71	0
2	YT3	B	2	1/1	1.00	0.14	65,65,65,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.