



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 03:50 PM EDT

PDB ID : 1U7V  
Title : Crystal Structure of the phosphorylated Smad2/Smad4 heterotrimeric complex  
Authors : Chacko, B.M.; Qin, B.Y.; Tiwari, A.; Shi, G.; Lam, S.; Hayward, L.J.; de Caestecker, M.; Lin, K.  
Deposited on : 2004-08-04  
Resolution : 2.70 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.35  
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

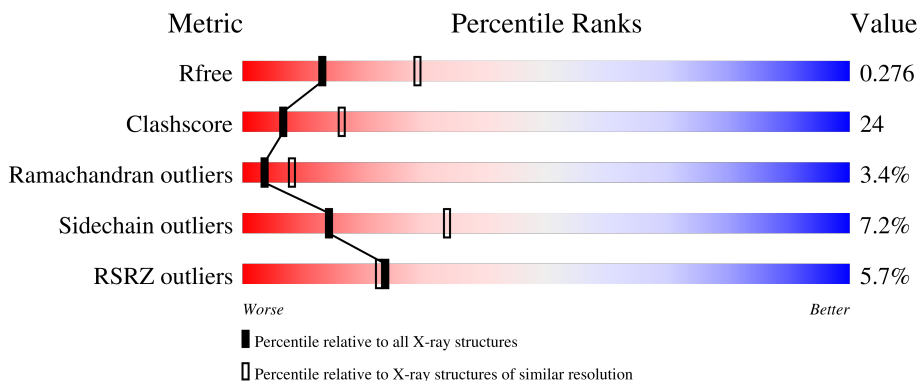
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

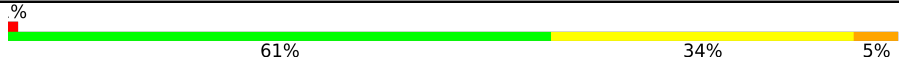
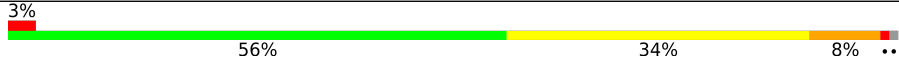

The reported resolution of this entry is 2.70 Å.

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	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  $\geq 3$ , 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	198	
1	C	198	
2	B	236	

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
1	SEP	A	467	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4777 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 Mothers against decapentaplegic homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	198	1574	987	277	294	2	14	0	0	0
1	C	196	1558	977	275	290	2	14	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	465	SEP	SER	modified residue	UNP Q15796
A	467	SEP	SER	modified residue	UNP Q15796
C	465	SEP	SER	modified residue	UNP Q15796
C	467	SEP	SER	modified residue	UNP Q15796

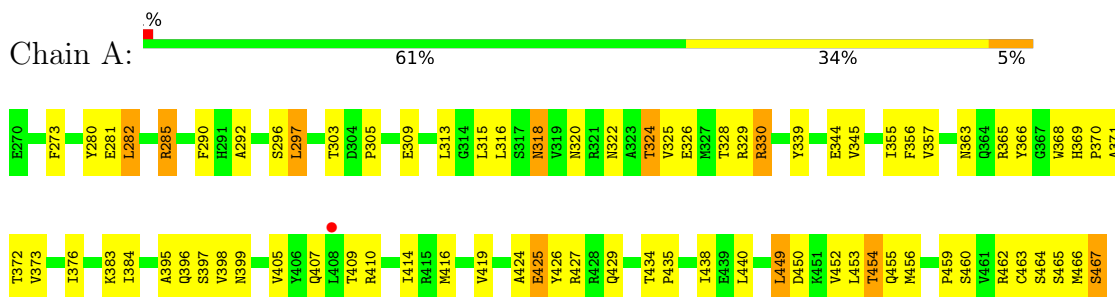
- Molecule 2 is a protein called Mothers against decapentaplegic homolog 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	208	1645	1038	295	300	12	0	0	0

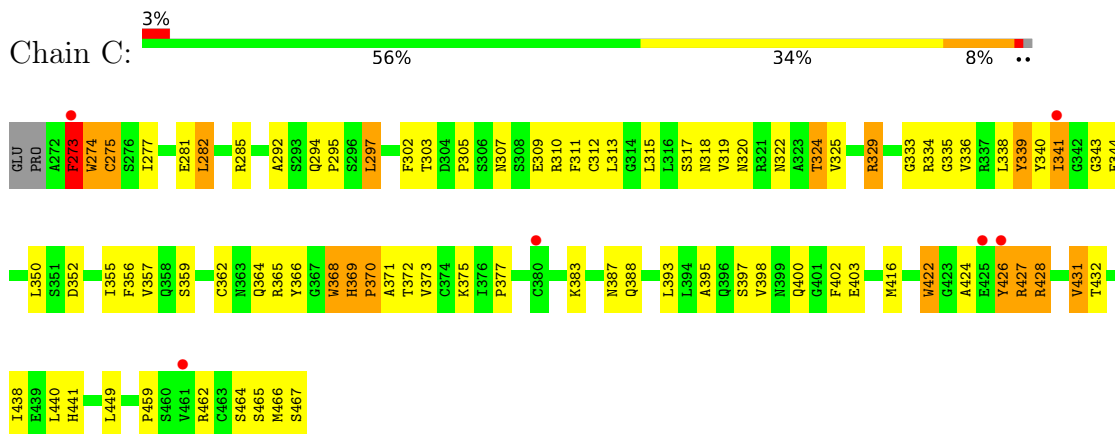
### 3 Residue-property plots [i](#)

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.

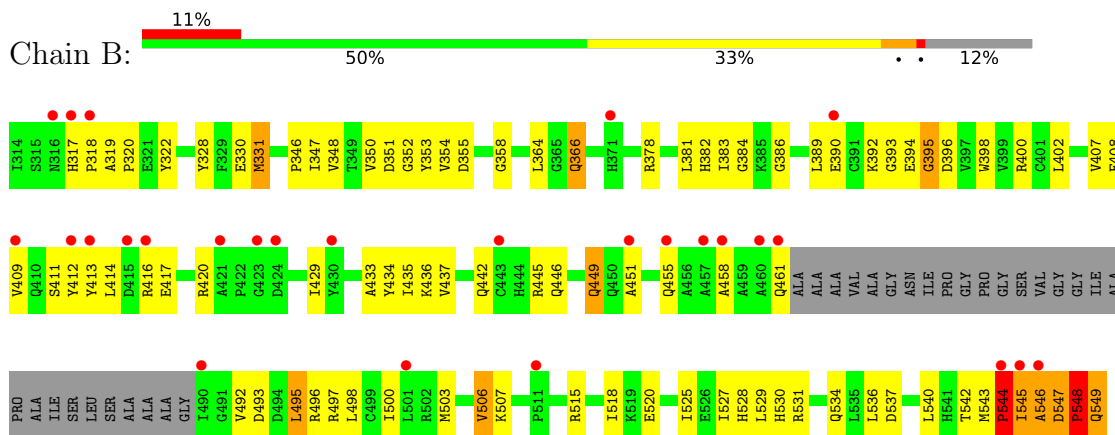
- Molecule 1: Mothers against decapentaplegic homolog 2



- Molecule 1: Mothers against decapentaplegic homolog 2



- Molecule 2: Mothers against decapentaplegic homolog 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.24Å 59.95Å 207.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.70 47.91 – 2.69	Depositor EDS
% Data completeness (in resolution range)	82.5 (100.00-2.70) 82.2 (47.91-2.69)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.69Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.243 , 0.279 0.235 , 0.276	Depositor DCC
$R_{free}$ test set	1485 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.3	Xtrriage
Anisotropy	0.212	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 61.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4777	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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

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	0.54	0/1592	0.67	0/2161
1	C	0.50	0/1575	0.74	2/2137 (0.1%)
2	B	0.46	0/1686	0.67	2/2287 (0.1%)
All	All	0.50	0/4853	0.70	4/6585 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	426	TYR	N-CA-C	-9.57	85.16	111.00
2	B	548	PRO	N-CA-C	5.79	127.16	112.10
2	B	547	ASP	C-N-CA	-5.78	97.71	122.00
1	C	428	ARG	N-CA-C	-5.07	97.32	111.00

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	1574	0	1511	67	0
1	C	1558	0	1499	81	0
2	B	1645	0	1601	92	0
All	All	4777	0	4611	221	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 24.

All (221) 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:339:TYR:CE1	1:C:341:ILE:HG12	2.04	0.93
1:C:368:TRP:CE3	1:C:372:THR:HG21	2.09	0.87
1:A:357:VAL:HG22	1:A:416:MET:HG2	1.56	0.86
2:B:545:ILE:HD12	2:B:545:ILE:H	1.44	0.83
1:A:384:ILE:CG2	1:A:414:ILE:HD13	2.10	0.82
2:B:545:ILE:O	2:B:547:ASP:N	2.14	0.81
1:C:273:PHE:O	1:C:275:CYS:N	2.14	0.80
1:C:336:VAL:HG21	1:C:416:MET:HE1	1.63	0.79
1:C:294:GLN:HG3	1:C:309:GLU:HG2	1.67	0.77
1:C:307:ASN:HB3	1:C:310:ARG:HB2	1.66	0.77
2:B:549:GLN:N	2:B:549:GLN:OE1	2.18	0.75
1:C:352:ASP:OD2	2:B:545:ILE:HG21	1.86	0.75
2:B:346:PRO:HG2	2:B:347:ILE:HD12	1.69	0.75
1:A:384:ILE:HG23	1:A:414:ILE:HD13	1.70	0.74
1:A:463:CYS:HB2	2:B:382:HIS:CD2	2.23	0.72
1:C:397:SER:HA	1:C:400:GLN:OE1	1.91	0.71
1:C:277:ILE:HG22	1:C:438:ILE:HG12	1.70	0.71
2:B:545:ILE:H	2:B:545:ILE:CD1	2.03	0.71
2:B:495:LEU:HD21	2:B:536:LEU:HD11	1.72	0.70
1:C:334:ARG:HB2	1:C:350:LEU:HB3	1.73	0.69
1:A:407:GLN:HE21	1:A:410:ARG:NH2	1.91	0.69
1:A:452:VAL:O	1:A:456:MET:HG2	1.94	0.68
1:C:368:TRP:HE3	1:C:372:THR:HG21	1.56	0.67
1:C:373:VAL:HG21	1:C:422:TRP:O	1.96	0.65
1:C:329:ARG:HB3	1:C:329:ARG:HH11	1.61	0.65
1:A:398:VAL:HG23	1:A:399:ASN:ND2	2.12	0.64
1:A:427:ARG:HG2	1:C:466:MET:HE3	1.78	0.64
2:B:347:ILE:HG13	2:B:390:GLU:HG3	1.78	0.64
1:C:281:GLU:O	1:C:282:LEU:HB2	1.98	0.64
2:B:400:ARG:HG2	2:B:402:LEU:CD1	2.26	0.64
1:C:359:SER:HB3	1:C:362:CYS:HB3	1.79	0.63
2:B:392:LYS:HD2	2:B:398:TRP:NE1	2.12	0.63
1:A:322:ASN:OD1	1:A:324:THR:HG23	1.98	0.63
1:C:339:TYR:HE1	1:C:341:ILE:HG12	1.59	0.62
1:A:313:LEU:O	1:A:329:ARG:NH2	2.33	0.62
1:C:343:GLY:CA	1:C:387:ASN:HD22	2.13	0.61
2:B:317:HIS:HB2	2:B:318:PRO:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:ILE:N	2:B:435:ILE:HD12	2.15	0.61
1:C:294:GLN:HG3	1:C:309:GLU:CG	2.32	0.60
2:B:544:PRO:O	2:B:545:ILE:C	2.40	0.60
1:A:407:GLN:HB3	1:A:410:ARG:NH2	2.18	0.59
1:A:281:GLU:O	1:A:282:LEU:HB2	2.01	0.59
1:C:302:PHE:O	1:C:312:CYS:HB3	2.03	0.59
2:B:433:ALA:HB1	2:B:435:ILE:CD1	2.32	0.58
2:B:392:LYS:HD2	2:B:398:TRP:CD1	2.38	0.58
1:C:322:ASN:ND2	1:C:324:THR:OG1	2.36	0.58
1:C:422:TRP:CZ2	1:C:431:VAL:HG13	2.38	0.58
1:C:375:LYS:HE2	1:C:377:PRO:HG3	1.85	0.58
2:B:350:VAL:HG13	2:B:364:LEU:HD11	1.84	0.57
1:C:277:ILE:HG23	1:C:440:LEU:HD12	1.87	0.56
2:B:328:TYR:HA	2:B:525:ILE:HG22	1.87	0.56
1:C:325:VAL:O	1:C:329:ARG:HG3	2.06	0.56
2:B:495:LEU:HD23	2:B:496:ARG:N	2.21	0.56
2:B:351:ASP:HB2	2:B:384:GLY:O	2.06	0.56
1:A:318:ASN:ND2	1:A:320:ASN:H	2.04	0.55
2:B:543:MET:O	2:B:544:PRO:C	2.45	0.55
1:C:319:VAL:HG23	1:C:320:ASN:ND2	2.22	0.54
1:C:355:ILE:HG13	1:C:355:ILE:O	2.07	0.54
2:B:407:VAL:HG23	2:B:429:ILE:HB	1.90	0.54
2:B:536:LEU:O	2:B:540:LEU:HG	2.07	0.54
2:B:451:ALA:HA	2:B:543:MET:CE	2.38	0.54
1:C:303:THR:O	1:C:305:PRO:HD3	2.08	0.54
2:B:346:PRO:O	2:B:390:GLU:HA	2.08	0.54
2:B:398:TRP:CZ2	2:B:436:LYS:HB2	2.43	0.54
1:C:369:HIS:O	1:C:371:ALA:N	2.41	0.54
2:B:451:ALA:O	2:B:455:GLN:HG3	2.08	0.53
2:B:458:ALA:HA	2:B:461:GLN:HE21	1.72	0.53
2:B:545:ILE:HD12	2:B:545:ILE:N	2.17	0.53
1:A:303:THR:O	1:A:305:PRO:HD3	2.08	0.53
1:C:329:ARG:HB3	1:C:329:ARG:NH1	2.24	0.53
1:A:339:TYR:O	1:A:345:VAL:HA	2.08	0.53
2:B:393:GLY:O	2:B:395:GLY:N	2.41	0.53
2:B:389:LEU:HD13	2:B:527:ILE:HD13	1.91	0.52
2:B:435:ILE:HG22	2:B:436:LYS:N	2.25	0.52
1:A:363:ASN:ND2	1:A:372:THR:HB	2.23	0.52
1:A:464:SER:OG	1:A:467:SEP:HB2	2.09	0.52
1:C:307:ASN:C	1:C:309:GLU:H	2.13	0.52
1:C:329:ARG:HD3	2:B:493:ASP:OD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:SER:CB	2:B:496:ARG:HH22	2.22	0.52
2:B:330:GLU:O	2:B:331:MET:HB2	2.09	0.51
1:C:422:TRP:CE2	1:C:431:VAL:HG13	2.45	0.51
1:C:364:GLN:HE22	1:C:393:LEU:HD22	1.76	0.51
1:C:368:TRP:O	1:C:369:HIS:C	2.48	0.51
1:A:326:GLU:HG3	1:A:330:ARG:HH21	1.75	0.51
1:A:454:THR:HA	2:B:353:TYR:CE2	2.46	0.51
1:C:302:PHE:HB3	2:B:537:ASP:OD2	2.10	0.51
1:C:313:LEU:O	1:C:329:ARG:NH2	2.43	0.50
2:B:411:SER:HB3	2:B:414:LEU:HD12	1.93	0.50
1:C:273:PHE:C	1:C:275:CYS:H	2.10	0.50
1:A:397:SER:C	1:A:399:ASN:N	2.64	0.50
1:C:402:PHE:CE1	1:C:459:PRO:HG3	2.47	0.50
1:A:463:CYS:SG	2:B:507:LYS:NZ	2.85	0.50
1:A:467:SEP:OG	1:A:467:SEP:O	2.26	0.50
1:C:426:TYR:O	1:C:428:ARG:N	2.43	0.50
1:A:397:SER:C	1:A:399:ASN:H	2.15	0.50
2:B:495:LEU:HD11	2:B:536:LEU:HD11	1.94	0.50
2:B:407:VAL:CG2	2:B:429:ILE:HB	2.41	0.49
1:C:285:ARG:HG2	1:C:285:ARG:HH11	1.75	0.49
2:B:545:ILE:O	2:B:546:ALA:C	2.51	0.49
1:A:315:LEU:HD12	1:A:316:LEU:N	2.26	0.49
2:B:492:VAL:HA	2:B:495:LEU:HD22	1.95	0.49
1:A:318:ASN:C	1:A:318:ASN:HD22	2.16	0.49
1:C:277:ILE:HG22	1:C:438:ILE:CG1	2.39	0.49
2:B:433:ALA:HB1	2:B:435:ILE:HD11	1.94	0.49
2:B:451:ALA:HA	2:B:543:MET:HE3	1.94	0.49
2:B:435:ILE:CG2	2:B:436:LYS:N	2.75	0.49
1:A:344:GLU:OE2	1:A:383:LYS:NZ	2.38	0.48
1:C:395:ALA:O	1:C:398:VAL:HG22	2.13	0.48
1:A:318:ASN:ND2	1:A:318:ASN:C	2.65	0.48
1:A:427:ARG:H	1:C:466:MET:CE	2.26	0.48
1:A:424:ALA:O	1:A:425:GLU:CB	2.62	0.48
2:B:393:GLY:C	2:B:395:GLY:H	2.17	0.48
1:C:356:PHE:N	1:C:356:PHE:CD1	2.81	0.48
1:A:407:GLN:HE21	1:A:410:ARG:HH22	1.60	0.48
1:C:333:GLY:C	1:C:335:GLY:H	2.15	0.48
2:B:378:ARG:O	2:B:381:LEU:HB2	2.14	0.48
2:B:496:ARG:NH1	2:B:500:ILE:HD11	2.29	0.48
1:A:453:LEU:C	1:A:455:GLN:H	2.17	0.48
1:C:277:ILE:CG2	1:C:438:ILE:HG12	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ASN:ND2	1:C:310:ARG:HD3	2.29	0.48
2:B:495:LEU:HD11	2:B:536:LEU:CD1	2.44	0.48
1:C:426:TYR:C	1:C:428:ARG:H	2.15	0.47
2:B:515:ARG:HH11	2:B:515:ARG:HG2	1.79	0.47
1:C:307:ASN:C	1:C:309:GLU:N	2.67	0.47
1:C:357:VAL:HG22	1:C:416:MET:HG2	1.95	0.47
1:A:281:GLU:HA	1:A:435:PRO:O	2.15	0.47
1:A:427:ARG:CG	1:C:466:MET:HE3	2.44	0.47
2:B:500:ILE:HD11	2:B:528:HIS:NE2	2.29	0.47
1:C:344:GLU:OE2	1:C:383:LYS:HD3	2.15	0.47
2:B:414:LEU:HD11	2:B:437:VAL:HG12	1.96	0.47
1:C:317:SER:HB2	2:B:496:ARG:HH22	1.79	0.47
1:A:427:ARG:H	1:C:466:MET:HE3	1.79	0.47
2:B:347:ILE:HD12	2:B:347:ILE:N	2.30	0.47
1:A:356:PHE:HB3	1:A:373:VAL:CG1	2.45	0.47
1:A:368:TRP:O	1:A:369:HIS:C	2.53	0.47
2:B:400:ARG:HA	2:B:433:ALA:O	2.14	0.47
2:B:446:GLN:O	2:B:449:GLN:HB3	2.14	0.46
1:C:365:ARG:HH12	1:C:383:LYS:HB3	1.80	0.46
1:C:366:TYR:HD2	1:C:368:TRP:CH2	2.34	0.46
1:C:307:ASN:CB	1:C:310:ARG:HB2	2.40	0.46
2:B:548:PRO:O	2:B:549:GLN:O	2.33	0.46
1:A:280:TYR:CE2	1:A:285:ARG:HG2	2.51	0.46
1:A:328:THR:HG23	1:A:419:VAL:HB	1.97	0.46
1:A:466:MET:O	1:A:467:SEP:OXT	2.34	0.46
1:C:329:ARG:HH11	1:C:329:ARG:CB	2.28	0.46
1:A:462:ARG:HG3	1:A:463:CYS:N	2.31	0.46
1:C:297:LEU:HD13	1:C:297:LEU:H	1.80	0.46
1:A:282:LEU:HD21	1:A:325:VAL:CG2	2.46	0.45
1:A:330:ARG:NH1	1:C:403:GLU:OE1	2.47	0.45
1:A:315:LEU:HD12	1:A:316:LEU:HD23	1.98	0.45
1:C:334:ARG:HH11	1:C:334:ARG:HG2	1.81	0.45
1:C:341:ILE:O	1:C:341:ILE:HG22	2.16	0.45
2:B:549:GLN:OE1	2:B:549:GLN:CA	2.64	0.45
1:C:311:PHE:CE1	1:C:438:ILE:HD11	2.52	0.45
2:B:400:ARG:HG2	2:B:402:LEU:HD12	1.98	0.45
2:B:434:TYR:C	2:B:435:ILE:HD12	2.38	0.45
1:A:355:ILE:CG1	1:A:376:ILE:HB	2.47	0.45
1:A:407:GLN:NE2	1:A:410:ARG:NH2	2.62	0.45
1:C:297:LEU:C	1:C:297:LEU:HD22	2.37	0.45
2:B:408:PHE:N	2:B:408:PHE:CD1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:409:VAL:HG22	2:B:503:MET:HG3	1.99	0.45
1:A:426:TYR:O	1:A:429:GLN:NE2	2.50	0.44
1:C:341:ILE:HD13	1:C:341:ILE:HA	1.84	0.44
2:B:400:ARG:HB2	2:B:434:TYR:HD1	1.83	0.44
2:B:320:PRO:HD3	2:B:534:GLN:OE1	2.17	0.44
2:B:545:ILE:C	2:B:547:ASP:N	2.70	0.44
1:A:273:PHE:HA	1:A:292:ALA:O	2.17	0.44
1:A:290:PHE:CE1	1:A:297:LEU:HD13	2.52	0.44
2:B:322:TYR:HB2	2:B:530:HIS:CE1	2.53	0.43
2:B:352:GLY:HA3	2:B:383:ILE:HB	2.01	0.43
1:A:450:ASP:CG	2:B:355:ASP:HB2	2.38	0.43
2:B:413:TYR:O	2:B:417:GLU:HG2	2.18	0.43
1:A:355:ILE:HG13	1:A:376:ILE:HB	2.00	0.43
2:B:398:TRP:CE2	2:B:436:LYS:HB2	2.54	0.43
1:A:325:VAL:O	1:A:329:ARG:HG3	2.18	0.43
1:C:282:LEU:O	1:C:432:THR:HA	2.17	0.43
1:C:333:GLY:C	1:C:335:GLY:N	2.72	0.43
2:B:435:ILE:N	2:B:435:ILE:CD1	2.81	0.43
1:A:467:SEP:OXT	2:B:515:ARG:NH2	2.52	0.43
2:B:366:GLN:HE21	2:B:366:GLN:HB2	1.54	0.43
1:A:297:LEU:HA	1:A:309:GLU:O	2.18	0.43
1:A:395:ALA:O	1:A:398:VAL:HG22	2.17	0.43
2:B:493:ASP:O	2:B:497:ARG:NH1	2.50	0.43
1:A:357:VAL:HG11	1:A:384:ILE:HG13	2.00	0.43
2:B:351:ASP:CG	2:B:353:TYR:HD1	2.23	0.43
1:A:366:TYR:HD1	1:A:368:TRP:CH2	2.38	0.42
1:A:395:ALA:C	1:A:397:SER:H	2.22	0.42
1:C:319:VAL:C	1:C:320:ASN:HD22	2.23	0.42
1:A:365:ARG:HD2	1:A:366:TYR:CE2	2.55	0.42
1:C:334:ARG:HH22	2:B:545:ILE:CD1	2.31	0.42
1:C:356:PHE:O	1:C:416:MET:HA	2.20	0.42
2:B:319:ALA:HA	2:B:531:ARG:NH1	2.34	0.42
2:B:548:PRO:C	2:B:549:GLN:O	2.57	0.42
1:A:464:SER:OG	1:A:467:SEP:CB	2.67	0.42
1:C:275:CYS:HA	1:C:441:HIS:O	2.19	0.42
2:B:536:LEU:O	2:B:536:LEU:HD12	2.20	0.41
2:B:542:THR:C	2:B:544:PRO:HD3	2.40	0.41
2:B:548:PRO:O	2:B:549:GLN:C	2.58	0.41
1:A:280:TYR:CZ	1:A:285:ARG:HG2	2.54	0.41
1:A:434:THR:HA	1:A:435:PRO:HD3	1.91	0.41
2:B:412:TYR:CE2	2:B:498:LEU:HD23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LEU:HD12	1:A:440:LEU:N	2.36	0.41
1:C:285:ARG:HG2	1:C:285:ARG:NH1	2.36	0.41
2:B:413:TYR:HE1	2:B:442:GLN:NE2	2.18	0.41
1:C:273:PHE:HA	1:C:292:ALA:O	2.21	0.41
1:C:281:GLU:O	1:C:282:LEU:CB	2.69	0.41
1:C:315:LEU:C	1:C:315:LEU:HD12	2.41	0.41
2:B:350:VAL:HG13	2:B:364:LEU:CD1	2.49	0.41
2:B:506:VAL:HG12	2:B:507:LYS:N	2.35	0.41
2:B:529:LEU:N	2:B:529:LEU:HD22	2.35	0.41
1:A:409:THR:CG2	2:B:354:VAL:HG11	2.51	0.40
2:B:384:GLY:C	2:B:386:GLY:H	2.24	0.40
1:A:405:VAL:HG12	1:A:449:LEU:HD21	2.03	0.40
1:C:294:GLN:HA	1:C:295:PRO:HD3	1.93	0.40
2:B:518:ILE:C	2:B:520:GLU:H	2.24	0.40
1:A:459:PRO:HB2	2:B:382:HIS:CE1	2.57	0.40
1:C:274:TRP:O	1:C:275:CYS:HB3	2.22	0.40
1:A:330:ARG:NH1	1:C:403:GLU:OE2	2.54	0.40
1:A:369:HIS:O	1:A:371:ALA:N	2.54	0.40
2:B:348:VAL:CG1	2:B:389:LEU:HB2	2.51	0.40
1:C:297:LEU:HD21	1:C:338:LEU:HD12	2.04	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	195/198 (98%)	178 (91%)	13 (7%)	4 (2%)	7	18
1	C	193/198 (98%)	170 (88%)	16 (8%)	7 (4%)	3	7
2	B	204/236 (86%)	175 (86%)	20 (10%)	9 (4%)	2	5
All	All	592/632 (94%)	523 (88%)	49 (8%)	20 (3%)	3	8

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	274	TRP
1	C	370	PRO
2	B	545	ILE
2	B	546	ALA
1	C	273	PHE
1	C	427	ARG
2	B	331	MET
2	B	358	GLY
2	B	506	VAL
2	B	544	PRO
1	C	282	LEU
2	B	548	PRO
1	A	282	LEU
1	A	454	THR
1	C	424	ALA
2	B	394	GLU
1	A	370	PRO
1	C	369	HIS
1	A	396	GLN
2	B	395	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	170/170 (100%)	160 (94%)	10 (6%)	19	43
1	C	168/170 (99%)	150 (89%)	18 (11%)	6	15
2	B	175/188 (93%)	166 (95%)	9 (5%)	24	50
All	All	513/528 (97%)	476 (93%)	37 (7%)	14	34

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	296	SER
1	A	297	LEU
1	A	318	ASN
1	A	324	THR
1	A	330	ARG
1	A	425	GLU
1	A	438	ILE
1	A	449	LEU
1	A	460	SER
1	C	273	PHE
1	C	275	CYS
1	C	297	LEU
1	C	318	ASN
1	C	324	THR
1	C	329	ARG
1	C	339	TYR
1	C	340	TYR
1	C	341	ILE
1	C	368	TRP
1	C	370	PRO
1	C	388	GLN
1	C	422	TRP
1	C	427	ARG
1	C	431	VAL
1	C	449	LEU
1	C	462	ARG
1	C	464	SER
2	B	366	GLN
2	B	396	ASP
2	B	416	ARG
2	B	420	ARG
2	B	445	ARG
2	B	449	GLN
2	B	495	LEU
2	B	544	PRO
2	B	549	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	284	GLN
1	A	318	ASN

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Mol	Chain	Res	Type
1	A	320	ASN
1	A	399	ASN
1	A	407	GLN
1	A	455	GLN
1	C	318	ASN
1	C	320	ASN
1	C	364	GLN
1	C	369	HIS
1	C	387	ASN
1	C	399	ASN
1	C	447	GLN
1	C	455	GLN
2	B	366	GLN
2	B	371	HIS
2	B	382	HIS
2	B	388	GLN
2	B	444	HIS
2	B	448	GLN
2	B	449	GLN
2	B	461	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](#)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEP	C	465	1	8,9,10	1.06	1 (12%)	8,12,14	1.75	2 (25%)
1	SEP	A	465	1	8,9,10	1.12	0	8,12,14	1.70	1 (12%)
1	SEP	A	467	1	9,10,10	1.09	1 (11%)	12,14,14	1.57	2 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEP	C	467	1	9,10,10	0.94	0	12,14,14	1.62	2 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	C	465	1	-	3/5/8/10	-
1	SEP	A	465	1	-	3/5/8/10	-
1	SEP	A	467	1	-	9/10/10/10	-
1	SEP	C	467	1	-	8/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	465	SEP	P-OG	2.67	1.68	1.60
1	A	467	SEP	P-OG	2.31	1.67	1.60

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	SEP	OG-P-O1P	3.27	115.64	106.47
1	C	465	SEP	OG-P-O1P	3.17	115.38	106.47
1	A	467	SEP	OG-P-O1P	3.14	115.28	106.47
1	C	467	SEP	OG-P-O1P	2.92	114.67	106.47
1	C	467	SEP	O2P-P-OG	2.13	112.41	106.73
1	A	467	SEP	O2P-P-OG	2.09	112.29	106.73
1	C	465	SEP	O2P-P-OG	2.06	112.21	106.73

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	465	SEP	CB-OG-P-O3P
1	A	467	SEP	N-CA-CB-OG
1	A	467	SEP	O-C-CA-CB
1	A	467	SEP	OXT-C-CA-CB
1	A	467	SEP	CB-OG-P-O3P
1	C	465	SEP	CB-OG-P-O3P

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Mol	Chain	Res	Type	Atoms
1	C	467	SEP	CB-OG-P-O1P
1	C	467	SEP	CB-OG-P-O3P
1	A	467	SEP	C-CA-CB-OG
1	C	467	SEP	O-C-CA-CB
1	A	467	SEP	CB-OG-P-O1P
1	A	467	SEP	O-C-CA-N
1	C	467	SEP	OXT-C-CA-CB
1	C	467	SEP	N-CA-CB-OG
1	C	467	SEP	C-CA-CB-OG
1	A	467	SEP	OXT-C-CA-N
1	A	465	SEP	CB-OG-P-O2P
1	A	467	SEP	CB-OG-P-O2P
1	C	465	SEP	CB-OG-P-O2P
1	C	467	SEP	CB-OG-P-O2P
1	A	465	SEP	CB-OG-P-O1P
1	C	465	SEP	CB-OG-P-O1P
1	C	467	SEP	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	467	SEP	5	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	196/198 (98%)	-0.02	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">92</span>	22, 46, 96, 108	0
1	C	194/198 (97%)	0.22	6 (3%) <span style="border: 1px solid gray; padding: 2px;">49</span> <span style="border: 1px solid gray; padding: 2px;">49</span>	35, 62, 93, 110	0
2	B	208/236 (88%)	0.71	27 (12%) <span style="border: 1px solid red; padding: 2px;">3</span> <span style="border: 1px solid red; padding: 2px;">2</span>	43, 82, 127, 136	0
All	All	598/632 (94%)	0.31	34 (5%) <span style="border: 1px solid red; padding: 2px;">23</span> <span style="border: 1px solid red; padding: 2px;">22</span>	22, 65, 114, 136	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	546	ALA	7.2
2	B	416	ARG	7.0
2	B	423	GLY	6.3
2	B	545	ILE	4.8
2	B	412	TYR	4.3
2	B	458	ALA	3.8
1	A	408	LEU	3.8
2	B	451	ALA	3.6
2	B	317	HIS	3.5
2	B	460	ALA	3.2
2	B	316	ASN	3.2
2	B	490	ILE	2.9
2	B	511	PRO	2.8
2	B	318	PRO	2.8
2	B	544	PRO	2.7
2	B	409	VAL	2.7
1	C	426	TYR	2.6
2	B	461	GLN	2.5
2	B	421	ALA	2.5
2	B	457	ALA	2.5
2	B	443	CYS	2.4
2	B	415	ASP	2.4
2	B	501	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	461	VAL	2.3
2	B	371	HIS	2.3
2	B	424	ASP	2.3
2	B	413	TYR	2.3
1	C	341	ILE	2.3
1	C	425	GLU	2.2
1	C	380	CYS	2.1
1	C	273	PHE	2.1
2	B	390	GLU	2.1
2	B	430	TYR	2.1
2	B	455	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	SEP	A	467	11/11	0.84	0.17	101,104,107,108	0
1	SEP	A	465	10/11	0.89	0.15	89,96,100,100	0
1	SEP	C	465	10/11	0.95	0.16	33,38,44,50	0
1	SEP	C	467	11/11	0.96	0.17	39,42,45,47	0

## 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.