Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:33 PM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

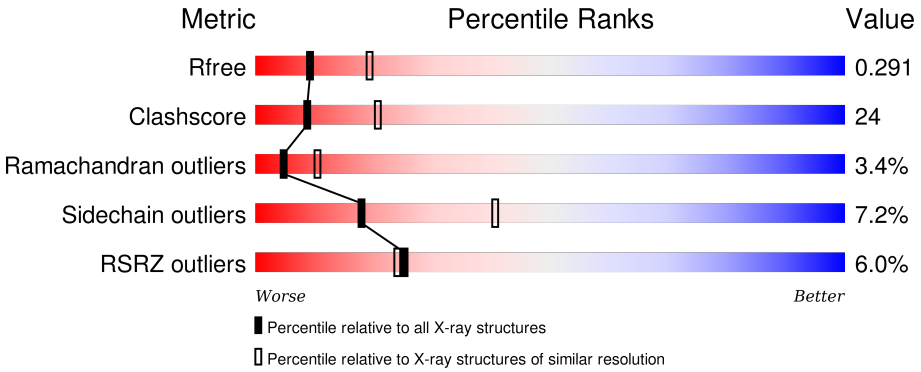
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 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	198	2% 61% 34% 5%
1	C	198	3% 57% 33% 8%
2	B	236	12% 50% 33% 12%

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
1	A	198	Total	C	N	O	P	S	0	0	0
			1574	987	277	294	2	14			
1	C	196	Total	C	N	O	P	S	0	0	0
			1558	977	275	290	2	14			

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.

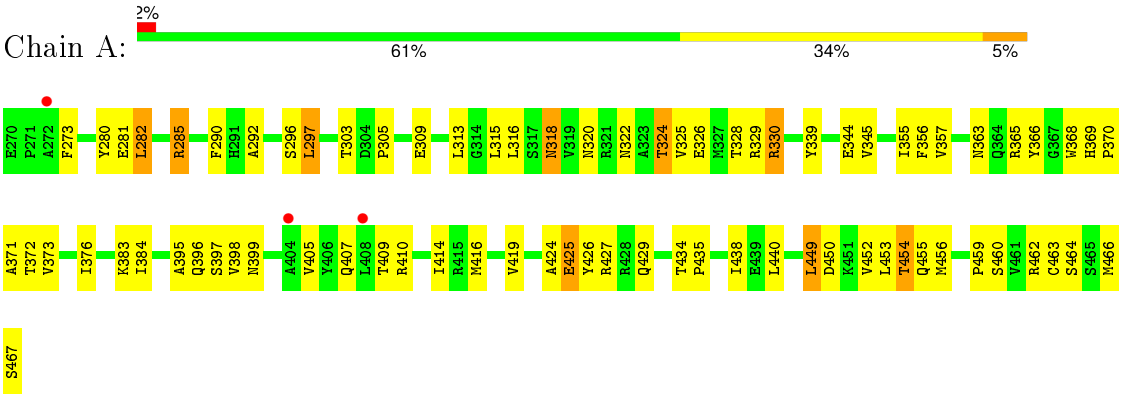
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1645	1038	295	300	12			

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.

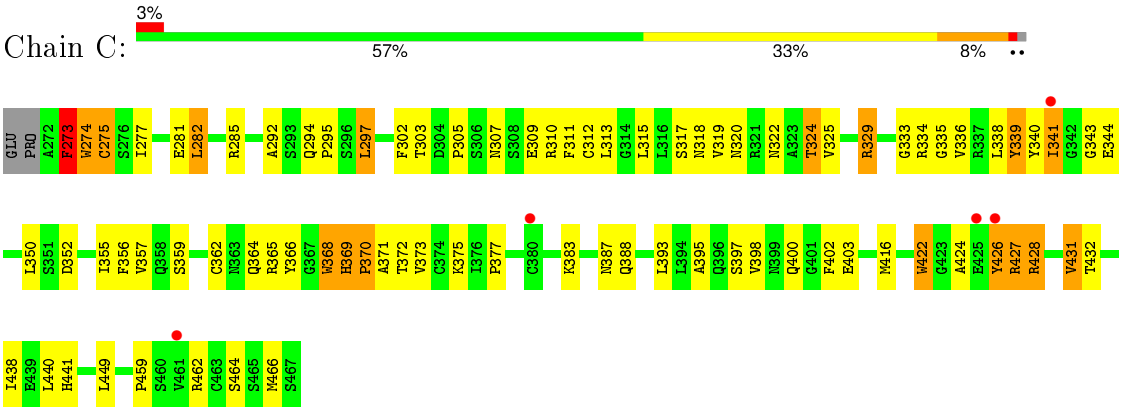
- Molecule 1: Mothers against decapentaplegic homolog 2

Chain A:



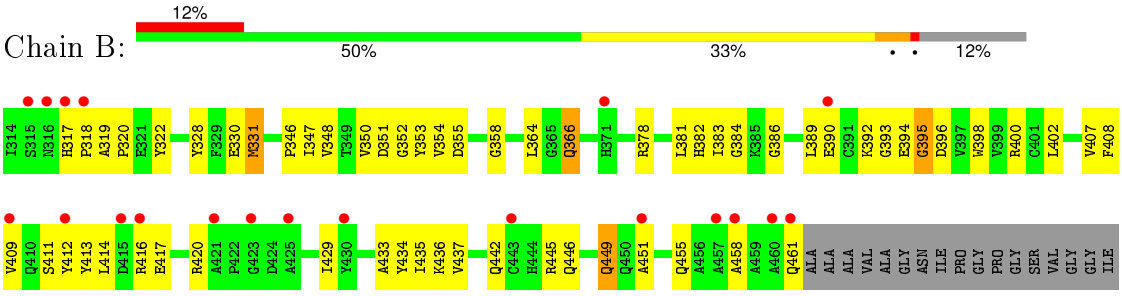
- Molecule 1: Mothers against decapentaplegic homolog 2

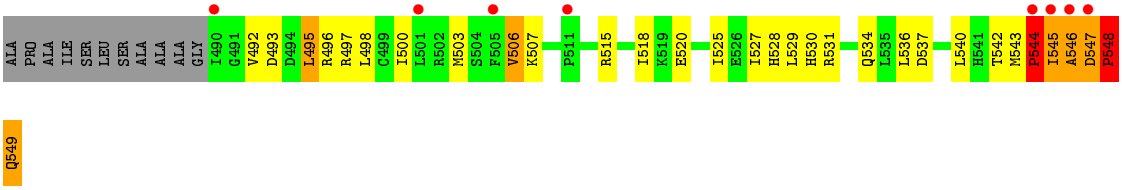
Chain C:



- Molecule 2: Mothers against decapentaplegic homolog 4

Chain B:




ALA
PRO
ALA
ILE
SER
LEU
SER
ALA
ALA
ALA
GLY
T490
G491
V492
D493
D494
L495
R496
R497
L498
C499
I500
L501
R502
M503
S504
F505
V506
K507
F511
R515
I518
K519
E520
I525
E526
I527
H528
L529
H530
R531
Q534
L535
L536
D537
L540
H541
T542
M543
P544
I545
A546
D547
P548
Q549

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.21 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.279 0.255 , 0.291	Depositor DCC
R_{free} test set	1485 reflections (10.21%)	DCC
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 15090 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4777	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage'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.*

[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: 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(^{o})	Ideal(^{o})
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

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:CD1	2:B:545:ILE:H	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:HH11	1:C:329:ARG:HB3	1.61	0.65
2:B:347:ILE:HG13	2:B:390:GLU:HG3	1.78	0.64
1:A:427:ARG:HG2	1:C:466:MET:HE3	1.78	0.64
1:A:398:VAL:HG23	1:A:399:ASN:ND2	2.12	0.64
2:B:400:ARG:HG2	2:B:402:LEU:CD1	2.26	0.64
1:C:281:GLU:O	1:C:282:LEU:HB2	1.98	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
2:B:317:HIS:HB2	2:B:318:PRO:HD2	1.81	0.61
1:C:343:GLY:CA	1:C:387:ASN:HD22	2.13	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
2:B:495:LEU:HD23	2:B:496:ARG:N	2.21	0.56
1:C:325:VAL:O	1:C:329:ARG:HG3	2.06	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
2:B:536:LEU:O	2:B:540:LEU:HG	2.07	0.54
2:B:407:VAL:HG23	2:B:429:ILE:HB	1.90	0.54
1:C:355:ILE:HG13	1:C:355:ILE:O	2.07	0.54
2:B:451:ALA:HA	2:B:543:MET:CE	2.38	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:303:THR:O	1:C:305:PRO:HD3	2.08	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:C:329:ARG:NH1	1:C:329:ARG:HB3	2.24	0.53
1:A:303:THR:O	1:A:305:PRO:HD3	2.08	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:C:307:ASN:C	1:C:309:GLU:H	2.13	0.52
1:A:464:SER:OG	1:A:467:SEP:HB2	2.09	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:O	1:A:467:SEP:OG	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:HH11	1:C:285:ARG:HG2	1.75	0.49
2:B:545:ILE:O	2:B:546:ALA:C	2.51	0.49
2:B:492:VAL:HA	2:B:495:LEU:HD22	1.95	0.49
1:A:315:LEU:HD12	1:A:316:LEU:N	2.26	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
1:A:318:ASN:C	1:A:318:ASN:HD22	2.16	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:C:395:ALA:O	1:C:398:VAL:HG22	2.13	0.48
1:A:344:GLU:OE2	1:A:383:LYS:NZ	2.38	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:CD1	1:C:356:PHE:N	2.81	0.48
2:B:496:ARG:NH1	2:B:500:ILE:HD11	2.29	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
1:C:307:ASN:ND2	1:C:310:ARG:HD3	2.29	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)
2:B:495:LEU:HD11	2:B:536:LEU:CD1	2.44	0.48
1:A:453:LEU:C	1:A:455:GLN:H	2.17	0.48
2:B:515:ARG:HH11	2:B:515:ARG:HG2	1.79	0.47
1:C:426:TYR:C	1:C:428:ARG:H	2.15	0.47
1:C:357:VAL:HG22	1:C:416:MET:HG2	1.95	0.47
1:C:307:ASN:C	1:C:309:GLU:N	2.67	0.47
2:B:500:ILE:HD11	2:B:528:HIS:NE2	2.29	0.47
1:A:427:ARG:CG	1:C:466:MET:HE3	2.44	0.47
1:A:281:GLU:HA	1:A:435:PRO:O	2.15	0.47
2:B:414:LEU:HD11	2:B:437:VAL:HG12	1.96	0.47
1:C:344:GLU:OE2	1:C:383:LYS:HD3	2.15	0.47
1:C:317:SER:HB2	2:B:496:ARG:HH22	1.79	0.47
2:B:347:ILE:N	2:B:347:ILE:HD12	2.30	0.47
1:A:427:ARG:H	1:C:466:MET:HE3	1.79	0.47
2:B:400:ARG:HA	2:B:433:ALA:O	2.14	0.47
1:A:368:TRP:O	1:A:369:HIS:C	2.53	0.47
1:A:356:PHE:HB3	1:A:373:VAL:CG1	2.45	0.47
2:B:446:GLN:O	2:B:449:GLN:HB3	2.14	0.46
1:C:366:TYR:HD2	1:C:368:TRP:CH2	2.34	0.46
1:C:365:ARG:HH12	1:C:383:LYS:HB3	1.80	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:C:329:ARG:HH11	1:C:329:ARG:CB	2.28	0.46
1:A:466:MET:O	1:A:467:SEP:OXT	2.34	0.46
1:A:328:THR:HG23	1:A:419:VAL:HB	1.97	0.46
1:A:280:TYR:CE2	1:A:285:ARG:HG2	2.51	0.46
1:A:462:ARG:HG3	1:A:463:CYS:N	2.31	0.46
1:C:297:LEU:H	1:C:297:LEU:HD13	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:C:341:ILE:HG22	1:C:341:ILE:O	2.16	0.45
1:C:334:ARG:HG2	1:C:334:ARG:HH11	1.81	0.45
1:A:315:LEU:HD12	1:A:316:LEU:HD23	1.98	0.45
2:B:549:GLN:CA	2:B:549:GLN:OE1	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:407:GLN:NE2	1:A:410:ARG:NH2	2.62	0.45
1:C:297:LEU:HD22	1:C:297:LEU:C	2.37	0.45
2:B:409:VAL:HG22	2:B:503:MET:HG3	1.99	0.45
1:A:355:ILE:CG1	1:A:376:ILE:HB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:PHE:CD1	2:B:408:PHE:N	2.85	0.45
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
1:A:426:TYR:O	1:A:429:GLN:NE2	2.50	0.44
2:B:545:ILE:C	2:B:547:ASP:N	2.70	0.44
2:B:320:PRO:HD3	2:B:534:GLN:OE1	2.17	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
2:B:398:TRP:CE2	2:B:436:LYS:HB2	2.54	0.43
1:A:355:ILE:HG13	1:A:376:ILE:HB	2.00	0.43
2:B:435:ILE:CD1	2:B:435:ILE:N	2.81	0.43
1:C:282:LEU:O	1:C:432:THR:HA	2.17	0.43
1:A:325:VAL:O	1:A:329:ARG:HG3	2.18	0.43
1:C:333:GLY:C	1:C:335:GLY:N	2.72	0.43
1:A:467:SEP:OXT	2:B:515:ARG:NH2	2.52	0.43
2:B:366:GLN:HB2	2:B:366:GLN:HE21	1.54	0.43
1:A:395:ALA:O	1:A:398:VAL:HG22	2.17	0.43
1:A:297:LEU:HA	1:A:309:GLU:O	2.18	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: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
1:A:365:ARG:HD2	1:A:366:TYR:CE2	2.55	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:C:275:CYS:HA	1:C:441:HIS:O	2.19	0.42
1:A:464:SER:OG	1:A:467:SEP:CB	2.67	0.42
2:B:536:LEU:HD12	2:B:536:LEU:O	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:C:285:ARG:NH1	1:C:285:ARG:HG2	2.36	0.41
2:B:413:TYR:HE1	2:B:442:GLN:NE2	2.18	0.41
1:A:440:LEU:N	1:A:440:LEU:HD12	2.36	0.41
1:C:273:PHE:HA	1:C:292:ALA:O	2.21	0.41
2:B:506:VAL:HG12	2:B:507:LYS:N	2.35	0.41
1:C:281:GLU:O	1:C:282:LEU:CB	2.69	0.41
2:B:350:VAL:HG13	2:B:364:LEU:CD1	2.49	0.41
2:B:529:LEU:N	2:B:529:LEU:HD22	2.35	0.41
1:C:315:LEU:C	1:C:315:LEU:HD12	2.41	0.41
2:B:384:GLY:C	2:B:386:GLY:H	2.24	0.40
1:A:409:THR:CG2	2:B:354:VAL:HG11	2.51	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:405:VAL:HG12	1:A:449:LEU:HD21	2.03	0.40
1:C:274:TRP:O	1:C:275:CYS:HB3	2.22	0.40
1:A:459:PRO:HB2	2:B:382:HIS:CE1	2.57	0.40
2:B:348:VAL:CG1	2:B:389:LEU:HB2	2.51	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
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%)	9 23
1	C	193/198 (98%)	170 (88%)	16 (8%)	7 (4%)	4 9
2	B	204/236 (86%)	175 (86%)	20 (10%)	9 (4%)	3 6
All	All	592/632 (94%)	523 (88%)	49 (8%)	20 (3%)	5 10

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

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%)	24 51
1	C	168/170 (99%)	150 (89%)	18 (11%)	8 19
2	B	175/188 (93%)	166 (95%)	9 (5%)	29 59
All	All	513/528 (97%)	476 (93%)	37 (7%)	18 41

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

Mol	Chain	Res	Type
1	A	285	ARG

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Mol	Chain	Res	Type
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

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

Mol	Chain	Res	Type
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

There are no RNA molecules in this entry.

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

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	A	465	1	8,9,10	1.12	0	8,12,14	1.84	2 (25%)
1	SEP	A	467	1	7,10,10	0.94	1 (14%)	7,14,14	1.93	2 (28%)
1	SEP	C	465	1	8,9,10	1.01	1 (12%)	8,12,14	1.91	3 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SEP	C	467	1	7,10,10	0.76	0	7,14,14	1.90	4 (57%)

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	A	465	1	-	0/6/8/10	0/0/0/0
1	SEP	A	467	1	-	0/6/10/10	0/0/0/0
1	SEP	C	465	1	-	0/6/8/10	0/0/0/0
1	SEP	C	467	1	-	0/6/10/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	467	SEP	P-OG	2.21	1.67	1.60
1	C	465	SEP	P-OG	2.55	1.68	1.60

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	467	SEP	O3P-P-O1P	-2.31	103.15	110.58
1	C	465	SEP	O3P-P-O1P	-2.30	103.16	110.58
1	A	465	SEP	O3P-P-O1P	-2.28	103.23	110.58
1	C	467	SEP	O3P-P-O1P	-2.20	103.49	110.58
1	C	465	SEP	O-C-CA	-2.02	120.24	125.49
1	C	467	SEP	O2P-P-OG	2.03	112.41	106.56
1	C	467	SEP	O2P-P-O1P	2.14	117.47	110.58
1	C	467	SEP	OG-P-O1P	2.96	114.67	107.14
1	A	467	SEP	OG-P-O1P	3.20	115.28	107.14
1	C	465	SEP	OG-P-O1P	3.24	115.38	107.14
1	A	465	SEP	OG-P-O1P	3.34	115.64	107.14

There are no chirality outliers.

There are no torsion outliers.

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	196/198 (98%)	-0.02	3 (1%) 76 76	22, 46, 96, 108	0
1	C	194/198 (97%)	0.23	5 (2%) 59 59	35, 62, 93, 110	0
2	B	208/236 (88%)	0.73	28 (13%) 4 3	43, 82, 127, 136	0
All	All	598/632 (94%)	0.32	36 (6%) 25 24	22, 65, 114, 136	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	416	ARG	7.5
2	B	546	ALA	7.3
2	B	423	GLY	6.0
2	B	545	ILE	4.9
2	B	412	TYR	4.8
2	B	458	ALA	3.9
2	B	317	HIS	3.7
2	B	451	ALA	3.6
1	A	408	LEU	3.5
2	B	316	ASN	3.4
2	B	460	ALA	3.0
2	B	457	ALA	2.9
2	B	461	GLN	2.8
2	B	318	PRO	2.8
2	B	490	ILE	2.7
2	B	409	VAL	2.6
2	B	544	PRO	2.6
2	B	511	PRO	2.6
2	B	371	HIS	2.6
1	C	425	GLU	2.6
2	B	421	ALA	2.5
1	C	461	VAL	2.4
2	B	501	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	443	CYS	2.3
1	C	380	CYS	2.3
2	B	415	ASP	2.3
1	C	426	TYR	2.3
1	C	341	ILE	2.2
2	B	430	TYR	2.1
2	B	390	GLU	2.1
2	B	547	ASP	2.1
2	B	315	SER	2.1
1	A	272	ALA	2.1
2	B	425	ALA	2.1
1	A	404	ALA	2.0
2	B	505	PHE	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. 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
1	SEP	A	465	10/11	0.90	0.15	-	89,96,100,100	0
1	SEP	A	467	11/11	0.85	0.16	-	101,104,107,108	0
1	SEP	C	467	11/11	0.97	0.16	-	39,42,45,47	0
1	SEP	C	465	10/11	0.96	0.16	-	33,38,44,50	0

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.