Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:50 PM GMT

PDB ID	:	4Q4J
Title	:	Structure of crosslinked TM287/288_S498C_S520C mutant
Authors	:	Hohl, M.; Schoeppe, J.; Gruetter, M.G.; Seeger, M.A.
Deposited on	:	2014-04-14
Resolution	:	3.20 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 ⓘ) were used in the production of this report:

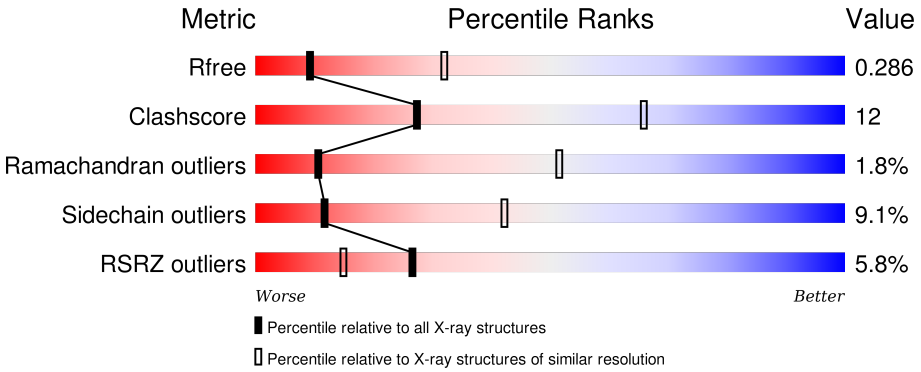
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	587	3% 65% 28% 5%
2	B	598	9% 65% 29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9126 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 ABC transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4485	2889	772	809	15			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	-8	PRO	-	EXPRESSION TAG	UNP Q9WYC3
A	-7	SER	-	EXPRESSION TAG	UNP Q9WYC3
A	-6	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	-5	SER	-	EXPRESSION TAG	UNP Q9WYC3
A	-4	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	-3	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	-2	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	-1	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	0	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	1	SER	-	EXPRESSION TAG	UNP Q9WYC3
A	28	SER	CYS	ENGINEERED MUTATION	UNP Q9WYC3
A	73	SER	CYS	ENGINEERED MUTATION	UNP Q9WYC3
A	496	SER	CYS	ENGINEERED MUTATION	UNP Q9WYC3
A	498	CYS	SER	ENGINEERED MUTATION	UNP Q9WYC3
A	519	SER	CYS	ENGINEERED MUTATION	UNP Q9WYC3
A	558	SER	CYS	ENGINEERED MUTATION	UNP Q9WYC3

- Molecule 2 is a protein called Uncharacterized ABC transporter ATP-binding protein TM_0288.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	583	Total	C	N	O	S	0	0	0
			4641	3000	782	844	15			

There is a discrepancy between the modelled and reference sequences:

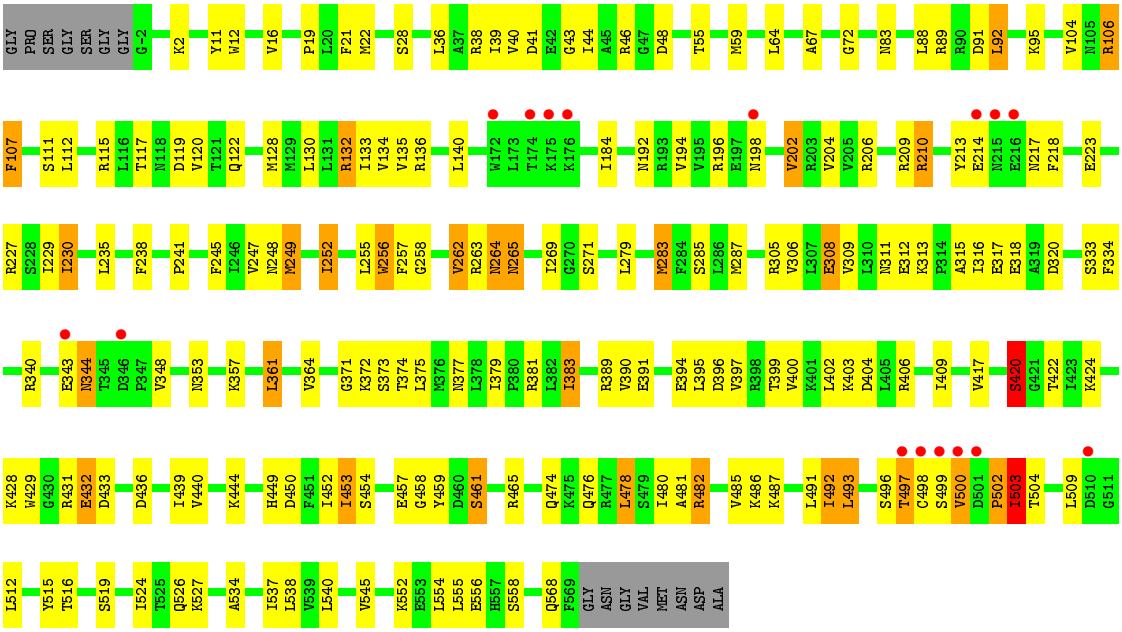
Chain	Residue	Modelled	Actual	Comment	Reference
B	520	CYS	SER	ENGINEERED MUTATION	UNP Q9WYC4

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.

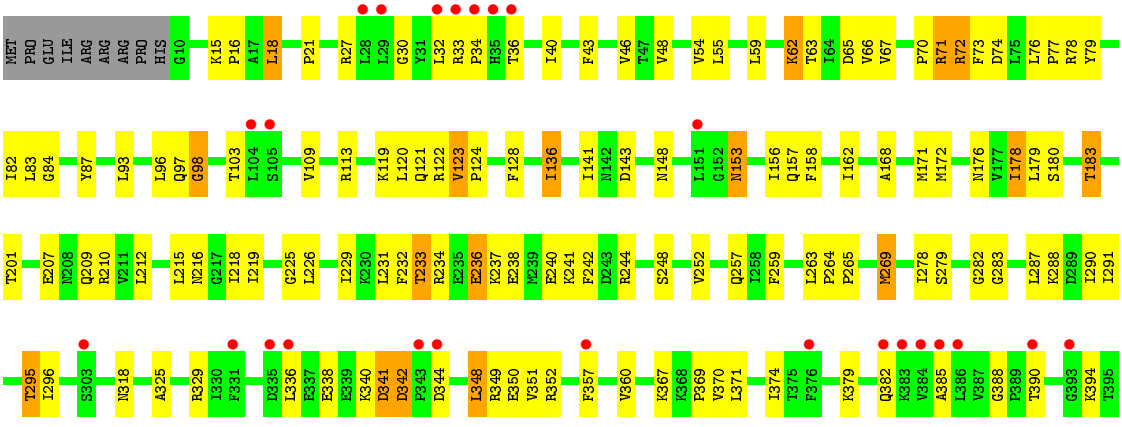
- Molecule 1: ABC transporter

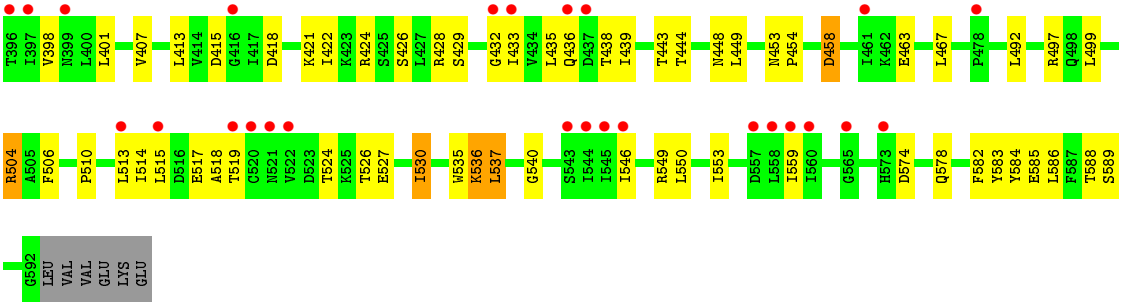
Chain A:



- Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM_0288

Chain B:




T396 I397 V398 N399 L400 L401 V407 L413 V414 D415 G416 I417 D418 K421 I422 K423 R424 S425 S426 L427 R428 S429 G432 I433 V434 L435 Q436 D437 T438 I439 T443 T444 N448 L449 N453 P454 D458 I461 K462 E463 L467 P478 L492 R497 Q498 L499
R504 A505 F506 P510 L513 I514 L515 D516 E517 A518 T519 C520 N521 V522 D523 T524 K525 T526 E527 I530 W535 K536 L537 G540 S543 I544 I545 I546 R549 L550 I553 D557 L558 I559 I560 G565 H573 D574 Q578 F582 Y583 Y584 E585 L586 F587 T588 S589
G592 LEU VAL VAL GLU LYS GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	216.67Å 84.14Å 113.46Å 90.00° 93.32° 90.00°	Depositor
Resolution (Å)	48.46 – 3.20 48.47 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.46-3.20) 98.7 (48.47-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.237 , 0.287 0.234 , 0.286	Depositor DCC
R_{free} test set	1671 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	109.0	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 61.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 33490 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9126	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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

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	0.44	0/4560	0.62	0/6166
2	B	0.35	0/4722	0.54	0/6385
All	All	0.40	0/9282	0.58	0/12551

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	4485	0	4682	122	0
2	B	4641	0	4828	126	0
All	All	9126	0	9510	222	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 12.

All (222) 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)
2:B:119:LYS:NZ	2:B:336:LEU:O	2.11	0.81
1:A:206:ARG:NH2	2:B:123:VAL:O	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LYS:NZ	1:A:312:GLU:O	2.13	0.79
1:A:38:ARG:HE	1:A:55:THR:HG21	1.49	0.76
1:A:92:LEU:HD21	1:A:306:VAL:HG13	1.68	0.73
2:B:122:ARG:HB3	2:B:338:GLU:HB3	1.69	0.73
1:A:526:GLN:NE2	2:B:519:THR:O	2.20	0.73
2:B:467:LEU:HB3	2:B:536:LYS:HD3	1.71	0.71
1:A:432:GLU:OE2	2:B:237:LYS:NZ	2.23	0.71
2:B:585:GLU:O	2:B:589:SER:OG	2.06	0.71
1:A:198:ASN:OD1	2:B:121:GLN:NE2	2.26	0.69
1:A:428:LYS:HE2	1:A:439:ILE:HD11	1.75	0.69
2:B:517:GLU:HB3	2:B:549:ARG:HH21	1.59	0.66
2:B:559:ILE:HG21	2:B:583:TYR:HE2	1.60	0.66
2:B:67:VAL:HG11	2:B:76:LEU:HD13	1.78	0.66
1:A:424:LYS:HB2	1:A:459:TYR:HB3	1.78	0.66
1:A:458:GLY:O	1:A:461:SER:HB3	1.96	0.65
1:A:361:LEU:HD23	1:A:534:ALA:HA	1.78	0.65
1:A:106:ARG:NH1	1:A:312:GLU:OE1	2.30	0.65
1:A:527:LYS:HA	1:A:568:GLN:HE22	1.62	0.64
1:A:230:ILE:HD11	2:B:103:THR:HA	1.78	0.64
2:B:418:ASP:HB3	2:B:421:LYS:HD2	1.77	0.64
1:A:40:VAL:HG12	1:A:44:ILE:HD12	1.78	0.64
2:B:388:GLY:O	2:B:394:LYS:NZ	2.25	0.64
1:A:449:HIS:HD1	1:A:459:TYR:HH	1.44	0.63
1:A:256:TRP:HD1	1:A:257:PHE:HD1	1.47	0.63
1:A:487:LYS:HA	1:A:515:TYR:OH	1.99	0.63
1:A:192:ASN:HB3	1:A:196:ARG:HH21	1.64	0.62
2:B:62:LYS:O	2:B:65:ASP:N	2.32	0.62
2:B:550:LEU:HD12	2:B:553:ILE:HD11	1.81	0.62
2:B:229:ILE:HG23	2:B:234:ARG:HB2	1.82	0.62
1:A:526:GLN:O	1:A:568:GLN:NE2	2.33	0.62
2:B:201:THR:OG1	2:B:259:PHE:O	2.18	0.62
2:B:70:PRO:O	2:B:72:ARG:N	2.32	0.61
2:B:527:GLU:OE2	2:B:549:ARG:NH1	2.33	0.61
1:A:204:VAL:HG21	2:B:439:ILE:HB	1.81	0.61
1:A:372:LYS:HA	1:A:540:LEU:HD12	1.82	0.61
2:B:72:ARG:NH1	2:B:74:ASP:OD2	2.35	0.60
2:B:398:VAL:HG22	2:B:514:ILE:HG21	1.84	0.60
1:A:89:ARG:HB2	1:A:120:VAL:HG11	1.83	0.60
1:A:184:ILE:HD13	1:A:229:ILE:HG12	1.83	0.60
1:A:452:ILE:HG21	1:A:459:TYR:CE1	2.36	0.60
2:B:219:ILE:HD11	2:B:242:PHE:HE2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLU:HB3	1:A:227:ARG:HH12	1.67	0.59
2:B:291:ILE:HB	2:B:295:THR:HG21	1.83	0.59
2:B:109:VAL:HG11	2:B:148:ASN:HB2	1.83	0.59
1:A:43:GLY:HA2	1:A:48:ASP:OD1	2.03	0.59
1:A:11:TYR:CZ	1:A:83:ASN:HB3	2.38	0.58
1:A:452:ILE:HG21	1:A:459:TYR:CD1	2.38	0.58
2:B:401:LEU:HD23	2:B:514:ILE:HD11	1.85	0.58
2:B:371:LEU:HD13	2:B:374:ILE:HG13	1.85	0.58
1:A:22:MET:SD	1:A:136:ARG:HB2	2.43	0.58
1:A:474:GLN:O	1:A:478:LEU:HB2	2.04	0.58
1:A:128:MET:HE2	2:B:257:GLN:HG3	1.86	0.58
2:B:18:LEU:HD22	2:B:21:PRO:HB3	1.85	0.58
1:A:256:TRP:CZ3	2:B:77:PRO:HG3	2.38	0.57
1:A:132:ARG:HD3	1:A:133:ILE:HG23	1.87	0.57
1:A:436:ASP:O	1:A:440:VAL:HG23	2.04	0.57
2:B:143:ASP:OD2	2:B:329:ARG:HD2	2.05	0.56
1:A:256:TRP:HD1	1:A:257:PHE:CD1	2.23	0.56
2:B:444:THR:O	2:B:448:ASN:ND2	2.37	0.56
1:A:245:PHE:O	1:A:249:MET:N	2.38	0.56
1:A:403:LYS:HG3	2:B:233:THR:HG21	1.87	0.56
2:B:229:ILE:HD13	2:B:238:GLU:HG3	1.86	0.56
2:B:78:ARG:O	2:B:82:ILE:HG13	2.05	0.56
1:A:256:TRP:HZ3	2:B:77:PRO:HG3	1.71	0.56
2:B:76:LEU:HB3	2:B:77:PRO:HD3	1.86	0.56
1:A:2:LYS:HG3	1:A:311:ASN:OD1	2.06	0.56
1:A:313:LYS:HE2	1:A:317:GLU:OE2	2.05	0.56
2:B:179:LEU:O	2:B:183:THR:HG23	2.06	0.55
2:B:176:ASN:OD1	2:B:178:ILE:HG12	2.06	0.55
1:A:258:GLY:O	1:A:262:VAL:HG12	2.07	0.54
1:A:509:LEU:HD23	1:A:512:LEU:HD12	1.89	0.54
2:B:59:LEU:HB3	2:B:83:LEU:HD11	1.89	0.54
2:B:584:TYR:CZ	2:B:588:THR:HG21	2.43	0.54
2:B:526:THR:O	2:B:530:ILE:HG23	2.08	0.53
1:A:364:VAL:HB	1:A:524:ILE:HG13	1.91	0.53
2:B:349:ARG:O	2:B:351:VAL:HG23	2.08	0.53
1:A:115:ARG:HD3	1:A:305:ARG:HB3	1.90	0.53
1:A:248:ASN:HB3	2:B:87:TYR:CD2	2.44	0.53
1:A:389:ARG:NH2	1:A:391:GLU:OE2	2.37	0.52
2:B:263:LEU:HB3	2:B:264:PRO:HD3	1.91	0.52
2:B:513:LEU:HD22	2:B:537:LEU:HD12	1.91	0.52
1:A:440:VAL:HG12	1:A:444:LYS:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLU:HB3	1:A:227:ARG:NH1	2.24	0.52
1:A:379:ILE:HG22	1:A:409:ILE:HD13	1.92	0.52
1:A:491:LEU:HD21	1:A:493:LEU:HD21	1.92	0.51
1:A:340:ARG:HA	1:A:348:VAL:HG23	1.93	0.51
1:A:38:ARG:NE	1:A:55:THR:HG21	2.22	0.51
1:A:371:GLY:O	1:A:374:THR:OG1	2.20	0.51
2:B:357:PHE:HD2	2:B:360:VAL:HG21	1.75	0.51
1:A:206:ARG:HG2	2:B:428:ARG:HH12	1.75	0.51
1:A:482:ARG:HD3	2:B:232:PHE:CZ	2.46	0.51
1:A:198:ASN:HB3	2:B:120:LEU:HD21	1.93	0.50
2:B:248:SER:O	2:B:252:VAL:HG23	2.11	0.50
2:B:59:LEU:HD23	2:B:83:LEU:HD12	1.94	0.50
2:B:379:LYS:O	2:B:382:GLN:HB2	2.12	0.49
1:A:117:THR:HG22	2:B:216:ASN:OD1	2.11	0.49
1:A:481:ALA:O	1:A:485:VAL:HG23	2.12	0.49
1:A:377:ASN:HB3	1:A:383:ILE:HD11	1.94	0.49
1:A:88:LEU:HD21	1:A:306:VAL:HG11	1.93	0.49
2:B:426:SER:O	2:B:429:SER:OG	2.26	0.49
1:A:238:PHE:O	1:A:241:PRO:HD2	2.13	0.49
2:B:236:GLU:O	2:B:240:GLU:HG3	2.13	0.49
2:B:433:ILE:HD11	2:B:435:LEU:HD21	1.94	0.49
1:A:202:VAL:O	1:A:206:ARG:HB2	2.11	0.49
1:A:420:SER:OG	1:A:465:ARG:HG2	2.12	0.48
2:B:66:VAL:HG11	2:B:79:TYR:CZ	2.47	0.48
1:A:476:GLN:O	1:A:480:ILE:HG13	2.14	0.48
1:A:344:ASN:N	1:A:344:ASN:OD1	2.46	0.48
1:A:263:ARG:HA	2:B:71:ARG:NH1	2.28	0.48
2:B:499:LEU:HG	2:B:530:ILE:HG22	1.95	0.48
2:B:109:VAL:O	2:B:113:ARG:HG3	2.14	0.48
2:B:264:PRO:HB2	2:B:265:PRO:HD3	1.94	0.48
1:A:452:ILE:O	1:A:458:GLY:HA2	2.13	0.48
2:B:517:GLU:HB3	2:B:549:ARG:NH2	2.27	0.48
2:B:449:LEU:HA	2:B:504:ARG:HB3	1.96	0.48
2:B:385:ALA:HB3	2:B:559:ILE:HG12	1.94	0.48
1:A:19:PRO:HB3	1:A:135:VAL:HG21	1.95	0.47
1:A:453:ILE:HA	1:A:453:ILE:HD12	1.67	0.47
2:B:48:VAL:HG23	2:B:93:LEU:HD13	1.96	0.47
2:B:153:ASN:OD1	2:B:157:GLN:HG3	2.13	0.47
1:A:202:VAL:HG11	2:B:128:PHE:HD2	1.80	0.47
1:A:450:ASP:O	1:A:453:ILE:HG22	2.14	0.47
1:A:512:LEU:O	1:A:516:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:ARG:HD2	2:B:210:ARG:HA	1.60	0.47
2:B:123:VAL:HG22	2:B:124:PRO:HD2	1.96	0.47
1:A:44:ILE:HD11	2:B:283:GLY:HA2	1.95	0.47
2:B:67:VAL:HG21	2:B:76:LEU:HA	1.97	0.47
1:A:263:ARG:C	1:A:265:ASN:H	2.17	0.47
1:A:502:PRO:HG2	1:A:504:THR:HG23	1.96	0.47
2:B:96:LEU:C	2:B:98:GLY:H	2.16	0.47
1:A:433:ASP:OD1	1:A:433:ASP:N	2.43	0.47
2:B:225:GLY:O	2:B:229:ILE:HG13	2.15	0.47
1:A:390:VAL:O	1:A:397:VAL:HG22	2.15	0.47
1:A:440:VAL:HG13	1:A:449:HIS:CE1	2.49	0.46
2:B:436:GLN:HG3	2:B:518:ALA:HB2	1.97	0.46
1:A:334:PHE:O	1:A:353:ASN:HA	2.15	0.46
2:B:582:PHE:O	2:B:586:LEU:HB2	2.15	0.46
1:A:417:VAL:O	1:A:482:ARG:NH2	2.48	0.46
1:A:252:ILE:HA	1:A:252:ILE:HD12	1.77	0.46
1:A:133:ILE:HA	1:A:136:ARG:HB3	1.97	0.46
1:A:397:VAL:O	1:A:400:VAL:HG22	2.16	0.46
1:A:104:VAL:HG21	2:B:226:LEU:HD23	1.98	0.46
1:A:486:LYS:NZ	2:B:231:LEU:O	2.46	0.46
1:A:214:GLU:HA	1:A:217:ASN:HB2	1.98	0.46
2:B:207:GLU:HG2	2:B:252:VAL:HG11	1.97	0.45
1:A:502:PRO:HB3	2:B:390:THR:H	1.81	0.45
1:A:21:PHE:CD2	1:A:72:GLY:HA3	2.51	0.45
2:B:287:LEU:HD23	2:B:287:LEU:HA	1.80	0.45
1:A:402:LEU:HD22	1:A:406:ARG:NH2	2.30	0.45
2:B:341:ASP:CG	2:B:424:ARG:H	2.19	0.45
1:A:449:HIS:ND1	1:A:459:TYR:OH	2.36	0.45
1:A:503:ILE:O	1:A:503:ILE:HD13	2.16	0.45
2:B:183:THR:HG22	2:B:278:ILE:HG12	1.98	0.45
1:A:389:ARG:HD2	1:A:396:ASP:OD2	2.17	0.45
2:B:236:GLU:HG2	2:B:236:GLU:H	1.48	0.45
1:A:209:ARG:NH1	2:B:429:SER:HA	2.33	0.44
2:B:394:LYS:HD2	2:B:546:ILE:HG23	2.00	0.44
2:B:66:VAL:HG11	2:B:79:TYR:CE1	2.53	0.44
2:B:342:ASP:HB3	2:B:344:ASP:OD1	2.18	0.44
2:B:527:GLU:CD	2:B:549:ARG:HH12	2.20	0.44
2:B:33:ARG:N	2:B:34:PRO:HD2	2.33	0.44
2:B:36:THR:O	2:B:40:ILE:HG12	2.18	0.44
1:A:315:ALA:O	1:A:316:ILE:HD13	2.18	0.44
1:A:67:ALA:HB2	2:B:269:MET:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:SER:O	1:A:115:ARG:HG3	2.16	0.44
1:A:21:PHE:HD2	1:A:72:GLY:HA3	1.83	0.43
1:A:39:ILE:HD12	2:B:279:SER:HB3	2.00	0.43
1:A:396:ASP:HB3	1:A:399:THR:OG1	2.18	0.43
1:A:107:PHE:HE2	1:A:308:GLU:HB3	1.82	0.43
1:A:428:LYS:HE2	1:A:439:ILE:CD1	2.47	0.43
2:B:453:ASN:HA	2:B:454:PRO:HD2	1.89	0.43
2:B:218:ILE:HD13	2:B:241:LYS:HD2	2.00	0.43
2:B:524:THR:O	2:B:527:GLU:HB3	2.19	0.43
2:B:352:ARG:NH1	2:B:540:GLY:O	2.52	0.43
2:B:515:LEU:HD22	2:B:517:GLU:HG2	2.01	0.42
2:B:530:ILE:HD11	2:B:549:ARG:NH2	2.33	0.42
2:B:71:ARG:O	2:B:73:PHE:N	2.50	0.42
1:A:136:ARG:CZ	1:A:140:LEU:HD11	2.48	0.42
1:A:40:VAL:HG23	1:A:41:ASP:OD1	2.20	0.42
2:B:288:LYS:HB3	2:B:290:ILE:HG13	2.00	0.42
2:B:55:LEU:HA	2:B:55:LEU:HD23	1.86	0.42
1:A:499:SER:HA	1:A:500:VAL:HA	1.39	0.42
1:A:210:ARG:HG3	1:A:213:TYR:HB3	2.01	0.42
2:B:168:ALA:O	2:B:172:MET:HB2	2.19	0.42
2:B:553:ILE:O	2:B:559:ILE:HD11	2.19	0.42
2:B:367:LYS:O	2:B:369:PRO:HD3	2.19	0.42
1:A:112:LEU:HD12	1:A:112:LEU:HA	1.65	0.42
1:A:92:LEU:HD12	1:A:309:VAL:HG12	2.02	0.42
2:B:158:PHE:O	2:B:162:ILE:HG12	2.19	0.42
1:A:379:ILE:HD12	1:A:492:ILE:HD13	2.01	0.42
1:A:130:LEU:HA	1:A:134:VAL:HB	2.02	0.42
2:B:492:LEU:O	2:B:497:ARG:NH1	2.52	0.42
1:A:194:VAL:HG11	1:A:218:PHE:HA	2.02	0.42
1:A:36:LEU:HD13	2:B:279:SER:OG	2.19	0.42
2:B:458:ASP:OD1	2:B:458:ASP:N	2.53	0.42
1:A:537:ILE:HB	1:A:554:LEU:CD1	2.49	0.41
2:B:16:PRO:HB2	2:B:325:ALA:HB2	2.03	0.41
1:A:496:SER:HA	1:A:497:THR:C	2.41	0.41
2:B:348:LEU:HD23	2:B:422:ILE:HG21	2.02	0.41
2:B:30:GLY:HA2	2:B:33:ARG:HD2	2.03	0.41
1:A:64:LEU:HA	1:A:64:LEU:HD23	1.86	0.41
2:B:413:LEU:HB3	2:B:418:ASP:HA	2.01	0.41
2:B:136:ILE:HA	2:B:136:ILE:HD13	1.66	0.41
1:A:11:TYR:CE2	1:A:83:ASN:HB3	2.55	0.41
2:B:341:ASP:OD2	2:B:424:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:LEU:O	2:B:212:LEU:HG	2.14	0.41
2:B:574:ASP:O	2:B:578:GLN:HB2	2.21	0.41
1:A:206:ARG:HG2	2:B:428:ARG:NH1	2.36	0.41
2:B:559:ILE:HG21	2:B:583:TYR:CE2	2.48	0.41
2:B:370:VAL:O	2:B:371:LEU:HD23	2.21	0.41
2:B:349:ARG:NH2	2:B:415:ASP:O	2.54	0.41
2:B:282:GLY:C	2:B:296:ILE:HD11	2.42	0.41
1:A:247:VAL:HG22	1:A:283:MET:HG3	2.03	0.41
1:A:12:TRP:O	1:A:16:VAL:HG13	2.20	0.40
1:A:457:GLU:OE2	1:A:457:GLU:N	2.54	0.40
2:B:15:LYS:HE3	2:B:318:ASN:OD1	2.21	0.40
2:B:291:ILE:HD12	2:B:295:THR:HG22	2.03	0.40
2:B:432:GLY:HA3	2:B:510:PRO:HG3	2.04	0.40
1:A:115:ARG:HA	1:A:119:ASP:OD2	2.22	0.40
1:A:16:VAL:C	1:A:19:PRO:HD2	2.42	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	570/587 (97%)	517 (91%)	41 (7%)	12 (2%)	9 46
2	B	581/598 (97%)	525 (90%)	47 (8%)	9 (2%)	13 55
All	All	1151/1185 (97%)	1042 (90%)	88 (8%)	21 (2%)	11 51

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	498	CYS
1	A	503	ILE
1	A	558	SER

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Mol	Chain	Res	Type
2	B	71	ARG
1	A	46	ARG
1	A	106	ARG
1	A	420	SER
2	B	63	THR
2	B	72	ARG
1	A	394	GLU
1	A	502	PRO
2	B	62	LYS
2	B	84	GLY
2	B	153	ASN
2	B	350	GLU
1	A	264	ASN
1	A	556	GLU
1	A	343	GLU
2	B	97	GLN
1	A	256	TRP
2	B	98	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	496/504 (98%)	440 (89%)	56 (11%)	7 31
2	B	518/533 (97%)	482 (93%)	36 (7%)	19 59
All	All	1014/1037 (98%)	922 (91%)	92 (9%)	12 42

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	59	MET
1	A	91	ASP
1	A	92	LEU
1	A	107	PHE

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Mol	Chain	Res	Type
1	A	122	GLN
1	A	132	ARG
1	A	202	VAL
1	A	210	ARG
1	A	230	ILE
1	A	235	LEU
1	A	249	MET
1	A	252	ILE
1	A	255	LEU
1	A	262	VAL
1	A	264	ASN
1	A	265	ASN
1	A	269	ILE
1	A	271	SER
1	A	279	LEU
1	A	283	MET
1	A	285	SER
1	A	287	MET
1	A	308	GLU
1	A	318	GLU
1	A	320	ASP
1	A	333	SER
1	A	344	ASN
1	A	357	LYS
1	A	361	LEU
1	A	373	SER
1	A	375	LEU
1	A	381	ARG
1	A	383	ILE
1	A	395	LEU
1	A	404	ASP
1	A	420	SER
1	A	422	THR
1	A	429	TRP
1	A	431	ARG
1	A	432	GLU
1	A	453	ILE
1	A	454	SER
1	A	461	SER
1	A	478	LEU
1	A	482	ARG
1	A	492	ILE

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Mol	Chain	Res	Type
1	A	493	LEU
1	A	497	THR
1	A	500	VAL
1	A	503	ILE
1	A	519	SER
1	A	538	LEU
1	A	545	VAL
1	A	552	LYS
1	A	555	LEU
2	B	18	LEU
2	B	27	ARG
2	B	32	LEU
2	B	43	PHE
2	B	46	VAL
2	B	54	VAL
2	B	123	VAL
2	B	136	ILE
2	B	141	ILE
2	B	156	ILE
2	B	171	MET
2	B	178	ILE
2	B	180	SER
2	B	183	THR
2	B	209	GLN
2	B	215	LEU
2	B	233	THR
2	B	236	GLU
2	B	244	ARG
2	B	269	MET
2	B	295	THR
2	B	340	LYS
2	B	341	ASP
2	B	342	ASP
2	B	348	LEU
2	B	407	VAL
2	B	438	THR
2	B	443	THR
2	B	458	ASP
2	B	463	GLU
2	B	504	ARG
2	B	506	PHE
2	B	530	ILE

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Mol	Chain	Res	Type
2	B	535	TRP
2	B	536	LYS
2	B	537	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	ASN

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

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	572/587 (97%)	0.10	16 (2%) 56 42	55, 87, 136, 166	0
2	B	583/598 (97%)	0.33	51 (8%) 13 7	54, 123, 160, 174	0
All	All	1155/1185 (97%)	0.22	67 (5%) 26 15	54, 101, 153, 174	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	SER	7.8
2	B	545	ILE	7.2
1	A	501	ASP	5.9
2	B	382	GLN	5.6
2	B	385	ALA	5.6
2	B	384	VAL	5.5
2	B	546	ILE	5.1
2	B	521	ASN	5.1
2	B	515	LEU	5.0
2	B	544	ILE	4.7
2	B	32	LEU	4.7
2	B	432	GLY	4.3
1	A	500	VAL	4.3
1	A	176	LYS	4.3
2	B	386	LEU	4.2
1	A	498	CYS	4.2
2	B	151	LEU	4.0
1	A	510	ASP	3.9
2	B	519	THR	3.9
2	B	376	PHE	3.8
2	B	336	LEU	3.8
2	B	520	CYS	3.7
1	A	343	GLU	3.7
2	B	34	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	383	LYS	3.4
2	B	357	PHE	3.3
2	B	436	GLN	3.2
2	B	343	PRO	3.1
2	B	399	ASN	3.1
2	B	33	ARG	3.0
2	B	335	ASP	3.0
1	A	172	TRP	3.0
2	B	565	GLY	2.9
2	B	416	GLY	2.9
2	B	559	ILE	2.9
2	B	573	HIS	2.9
2	B	344	ASP	2.8
2	B	393	GLY	2.8
1	A	175	LYS	2.8
2	B	29	LEU	2.7
1	A	198	ASN	2.7
2	B	396	THR	2.6
2	B	36	THR	2.6
2	B	437	ASP	2.5
2	B	557	ASP	2.5
2	B	560	ILE	2.4
2	B	543	SER	2.4
2	B	461	ILE	2.4
2	B	478	PRO	2.4
1	A	214	GLU	2.3
1	A	174	THR	2.3
2	B	397	ILE	2.3
2	B	28	LEU	2.3
1	A	216	GLU	2.3
1	A	215	ASN	2.2
1	A	497	THR	2.2
2	B	35	HIS	2.2
2	B	331	PHE	2.2
2	B	433	ILE	2.2
2	B	513	LEU	2.1
2	B	522	VAL	2.1
2	B	105	SER	2.1
2	B	303	SER	2.0
2	B	558	LEU	2.0
1	A	346	ASP	2.0
2	B	390	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	104	LEU	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.