



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:04 AM GMT

PDB ID : 2FJI
Title : Crystal structure of the C-terminal domain of the exocyst subunit Sec6p
Authors : Sivaram, M.V.; Munson, M.
Deposited on : 2006-01-02
Resolution : 2.40 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

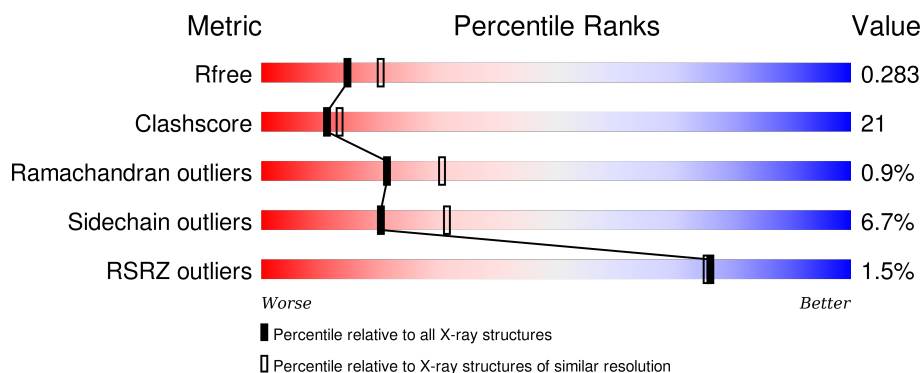
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

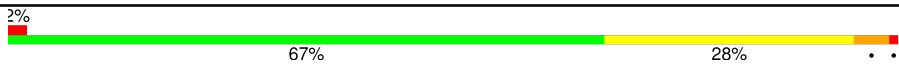
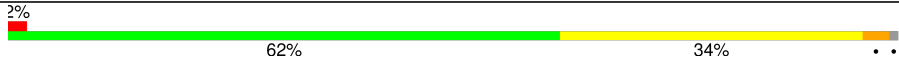
The reported resolution of this entry is 2.40 Å.

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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 $\leq 5\%$. 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	1	399	
1	2	399	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6868 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 Exocyst complex component SEC6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	399	Total	C	N	O	S	34	0	0
			3178	2027	516	617	18			
1	2	396	Total	C	N	O	S	59	0	0
			3076	1961	497	601	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	407	GLY	-	CLONING ARTIFACT	UNP P32844
1	408	SER	-	CLONING ARTIFACT	UNP P32844
1	409	HIS	-	CLONING ARTIFACT	UNP P32844
1	410	MET	-	CLONING ARTIFACT	UNP P32844
2	407	GLY	-	CLONING ARTIFACT	UNP P32844
2	408	SER	-	CLONING ARTIFACT	UNP P32844
2	409	HIS	-	CLONING ARTIFACT	UNP P32844
2	410	MET	-	CLONING ARTIFACT	UNP P32844

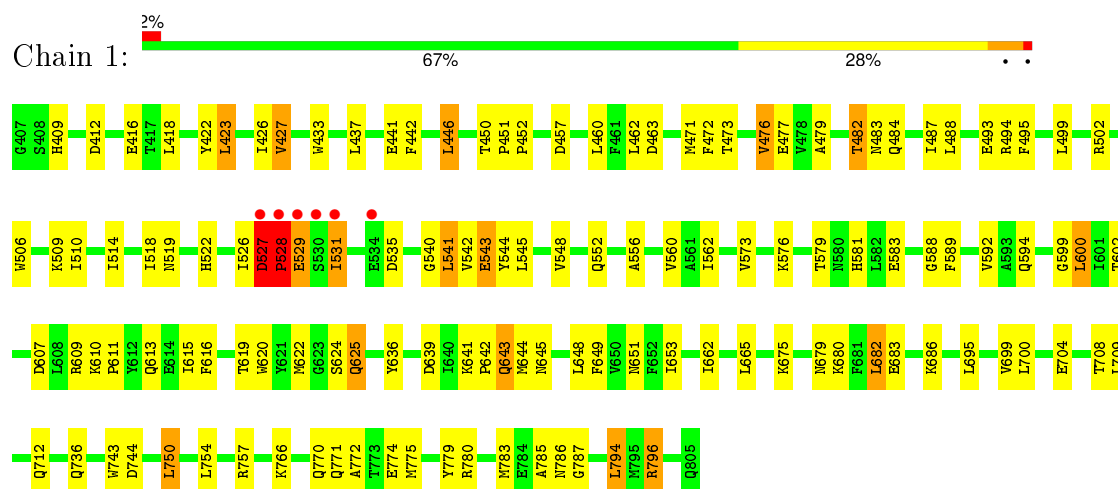
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	448	Total	O	0	0
			448	448		
2	2	166	Total	O	0	0
			166	166		

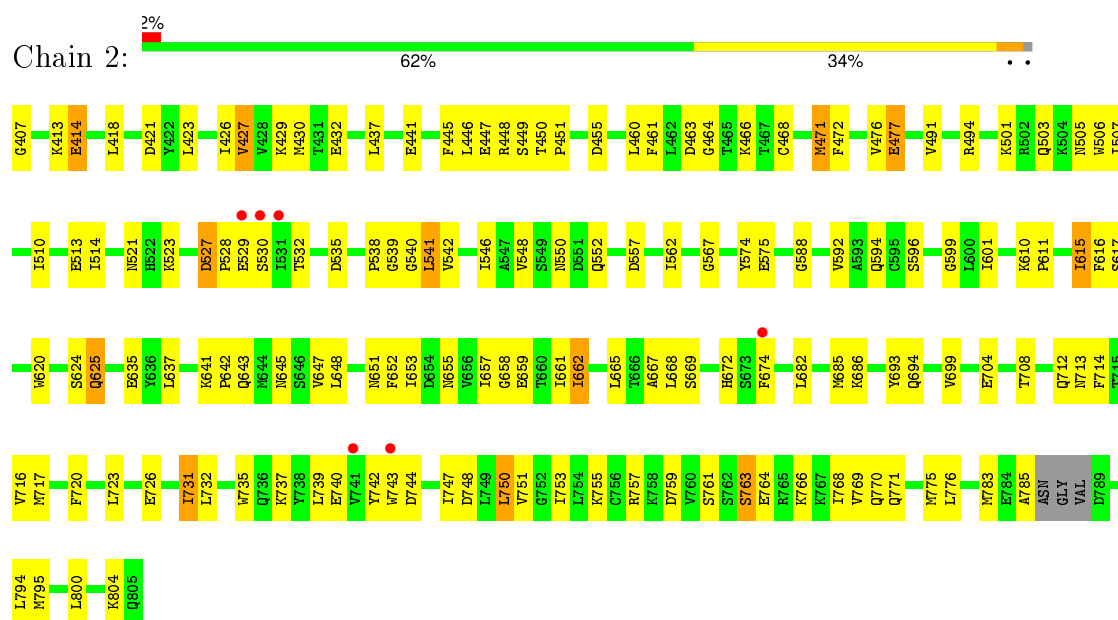
3 Residue-property plots

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: Exocyst complex component SEC6



• Molecule 1: Exocyst complex component SEC6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.30Å 63.30Å 151.47Å 90.00° 103.89° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 48.64 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.4 (15.00-2.40) 97.4 (48.64-2.38)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.284 0.251 , 0.283	Depositor DCC
R_{free} test set	3870 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.719	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 78645 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6868	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1	0.40	0/3237	0.57	0/4371
1	2	0.35	0/3134	0.53	0/4236
All	All	0.38	0/6371	0.55	0/8607

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	1	3178	0	3086	114	0
1	2	3076	0	2899	134	0
2	1	448	0	0	25	2
2	2	166	0	0	21	0
All	All	6868	0	5985	248	2

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 21.

All (248) 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)
1:2:448:ARG:HH12	1:2:538:PRO:HG2	1.19	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:619:THR:HB	2:1:1216:HOH:O	1.58	1.01
1:1:644:MET:CE	1:1:649:PHE:HA	2.04	0.87
1:2:693:TYR:HA	1:2:714:PHE:HE1	1.41	0.85
1:1:609:ARG:HD2	2:1:983:HOH:O	1.77	0.84
1:2:448:ARG:NH1	1:2:538:PRO:HG2	1.94	0.82
1:2:769:VAL:HG11	2:2:821:HOH:O	1.78	0.81
1:2:732:LEU:HD21	2:2:905:HOH:O	1.81	0.80
1:2:616:PHE:HE2	1:2:685:MET:HE1	1.46	0.79
1:1:482:THR:HG22	1:1:484:GLN:H	1.48	0.78
1:1:427:VAL:HG13	1:1:494:ARG:CZ	2.14	0.76
1:1:796:ARG:HH11	1:1:796:ARG:HB2	1.50	0.75
1:1:540:GLY:O	1:1:543:GLU:HG2	1.87	0.75
1:2:668:LEU:HD11	1:2:720:PHE:HE1	1.50	0.75
1:1:427:VAL:HG13	1:1:494:ARG:NH1	2.02	0.74
1:1:528:PRO:HA	1:1:531:ILE:HG23	1.68	0.74
1:2:658:GLY:O	1:2:662:ILE:HG23	1.88	0.74
1:1:441:GLU:HG3	2:1:1226:HOH:O	1.88	0.73
1:2:661:ILE:HD11	1:2:714:PHE:CD2	2.23	0.73
1:1:775:MET:SD	2:1:972:HOH:O	2.47	0.73
1:2:616:PHE:CE2	1:2:685:MET:HE1	2.24	0.73
1:2:616:PHE:HE2	1:2:685:MET:CE	2.01	0.72
1:2:427:VAL:HG13	1:2:494:ARG:NH1	2.06	0.71
1:1:662:ILE:HD11	1:1:794:LEU:HD22	1.72	0.70
1:2:507:ILE:HG13	1:2:592:VAL:HG22	1.73	0.70
1:1:736:GLN:HB2	1:1:775:MET:CE	2.21	0.70
1:2:739:LEU:HD21	1:2:776:LEU:HA	1.73	0.70
1:1:787:GLY:HA2	2:1:842:HOH:O	1.90	0.70
1:1:594:GLN:HE22	1:1:651:ASN:ND2	1.90	0.70
1:1:744:ASP:OD1	1:1:796:ARG:NH1	2.25	0.69
1:2:527:ASP:C	1:2:529:GLU:H	1.94	0.69
1:1:653:ILE:HG21	1:1:700:LEU:HD21	1.74	0.69
1:1:463:ASP:HB3	2:1:1195:HOH:O	1.92	0.69
1:2:427:VAL:HG13	1:2:494:ARG:CZ	2.23	0.69
1:1:675:LYS:HB2	1:1:680:LYS:HE3	1.72	0.69
1:2:716:VAL:HG21	1:2:795:MET:SD	2.33	0.69
1:2:763:SER:HB3	2:2:884:HOH:O	1.93	0.68
1:2:771:GLN:O	1:2:775:MET:HG3	1.92	0.68
1:2:694:GLN:HE21	1:2:694:GLN:HA	1.59	0.68
1:2:794:LEU:HD23	1:2:794:LEU:H	1.58	0.68
1:1:479:ALA:O	1:1:482:THR:HB	1.95	0.67
1:2:510:ILE:HD13	1:2:596:SER:HB3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:736:GLN:HB2	1:1:775:MET:HE2	1.77	0.67
1:2:737:LYS:HA	1:2:740:GLU:HG3	1.77	0.66
1:2:661:ILE:HD11	1:2:714:PHE:HD2	1.61	0.66
1:1:527:ASP:O	1:1:529:GLU:N	2.28	0.66
1:2:527:ASP:O	1:2:529:GLU:N	2.28	0.66
1:1:482:THR:HG21	1:1:487:ILE:HD12	1.75	0.66
1:2:542:VAL:O	1:2:546:ILE:HG13	1.96	0.66
1:2:742:TYR:CD2	1:2:795:MET:HG2	2.31	0.65
1:1:579:THR:O	1:1:583:GLU:HG3	1.96	0.65
1:1:518:ILE:HD11	1:1:602:THR:HG22	1.78	0.65
1:2:708:THR:O	1:2:712:GLN:HG2	1.96	0.65
1:2:599:GLY:HA2	2:2:937:HOH:O	1.97	0.65
1:1:473:THR:O	1:1:477:GLU:HG2	1.98	0.64
1:2:735:TRP:CZ2	1:2:747:ILE:HD12	2.33	0.64
1:1:441:GLU:HG2	1:1:506:TRP:HZ2	1.62	0.64
1:1:610:LYS:O	1:1:613:GLN:HG2	1.98	0.63
1:2:726:GLU:O	1:2:757:ARG:NH2	2.31	0.63
1:1:514:ILE:CD1	1:1:599:GLY:HA3	2.28	0.63
1:2:739:LEU:HD21	1:2:776:LEU:HD12	1.79	0.62
1:1:645:ASN:HD22	1:1:648:LEU:H	1.46	0.62
1:2:510:ILE:HD11	1:2:548:VAL:HG11	1.82	0.62
1:2:615:ILE:HG12	1:2:616:PHE:N	2.14	0.61
1:1:528:PRO:HA	1:1:531:ILE:CG2	2.30	0.61
1:2:472:PHE:CZ	1:2:476:VAL:HG11	2.35	0.61
1:2:472:PHE:CE2	1:2:562:ILE:HD13	2.36	0.61
1:1:639:ASP:O	1:1:642:PRO:HD2	2.01	0.61
1:2:735:TRP:CE3	1:2:750:LEU:HG	2.35	0.61
1:1:472:PHE:O	1:1:476:VAL:HG22	2.00	0.61
1:1:772:ALA:HA	2:1:972:HOH:O	2.00	0.60
1:2:546:ILE:HG22	1:2:550:ASN:HD21	1.65	0.60
1:1:622:MET:HE1	2:1:898:HOH:O	2.01	0.60
1:1:493:GLU:HG3	1:1:581:HIS:CE1	2.36	0.60
1:1:531:ILE:HG13	1:1:535:ASP:HB2	1.83	0.60
1:2:668:LEU:HD11	1:2:720:PHE:CE1	2.34	0.60
1:2:694:GLN:NE2	1:2:694:GLN:HA	2.16	0.60
1:2:441:GLU:HG2	1:2:506:TRP:HZ2	1.67	0.59
1:1:679:ASN:O	1:1:683:GLU:HG3	2.03	0.59
1:2:732:LEU:HB2	2:2:935:HOH:O	2.02	0.59
1:2:514:ILE:CD1	1:2:599:GLY:HA3	2.32	0.59
1:2:615:ILE:O	1:2:616:PHE:HB2	2.04	0.58
1:1:527:ASP:OD2	1:1:528:PRO:HD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:780:ARG:HD2	2:1:998:HOH:O	2.03	0.58
1:1:514:ILE:HD13	1:1:599:GLY:HA3	1.85	0.58
1:1:472:PHE:CZ	1:1:476:VAL:HG13	2.39	0.58
1:2:645:ASN:HD21	1:2:647:VAL:HB	1.69	0.58
1:2:472:PHE:CZ	1:2:476:VAL:CG1	2.86	0.58
1:1:708:THR:O	1:1:712:GLN:HG2	2.03	0.58
1:1:750:LEU:HD22	1:1:754:LEU:HG	1.86	0.57
1:1:509:LYS:HE2	2:1:1209:HOH:O	2.04	0.57
1:1:422:TYR:CZ	1:1:426:ILE:HD11	2.40	0.57
1:2:472:PHE:O	1:2:476:VAL:HG22	2.04	0.57
1:2:532:THR:H	1:2:535:ASP:HB2	1.70	0.57
1:1:624:SER:OG	2:1:806:HOH:O	2.18	0.57
1:2:764:GLU:O	1:2:768:ILE:HG13	2.05	0.57
1:1:482:THR:HG22	1:1:484:GLN:N	2.19	0.56
1:2:471:MET:HE2	2:2:966:HOH:O	2.05	0.56
1:1:796:ARG:HH11	1:1:796:ARG:CB	2.19	0.56
1:1:766:LYS:O	1:1:770:GLN:HG3	2.05	0.56
1:1:519:ASN:HA	2:1:1157:HOH:O	2.06	0.56
1:1:441:GLU:HA	2:1:1226:HOH:O	2.06	0.55
1:2:743:TRP:CZ3	1:2:744:ASP:HB3	2.41	0.55
1:2:624:SER:HA	2:2:808:HOH:O	2.06	0.55
1:1:644:MET:HE3	1:1:649:PHE:HA	1.87	0.55
1:2:514:ILE:HD13	1:2:599:GLY:HA3	1.88	0.55
1:1:452:PRO:HD3	1:1:544:TYR:CE1	2.41	0.55
1:1:437:LEU:O	1:1:441:GLU:HB2	2.07	0.55
1:2:748:ASP:HB3	1:2:800:LEU:HB3	1.89	0.55
1:1:427:VAL:CG1	1:1:494:ARG:CZ	2.85	0.55
1:1:771:GLN:C	2:1:972:HOH:O	2.46	0.54
1:1:779:TYR:O	1:1:783:MET:HG3	2.07	0.54
1:2:521:ASN:C	1:2:523:LYS:H	2.09	0.54
1:1:775:MET:CG	2:1:972:HOH:O	2.55	0.54
1:1:472:PHE:CE2	1:1:562:ILE:HD13	2.42	0.54
1:1:433:TRP:CD2	1:1:471:MET:HG3	2.42	0.54
1:1:541:LEU:HD22	1:1:545:LEU:HG	1.89	0.54
1:2:713:ASN:O	1:2:716:VAL:HG12	2.07	0.54
1:2:645:ASN:ND2	1:2:648:LEU:H	2.05	0.54
1:1:514:ILE:HD13	1:1:599:GLY:CA	2.38	0.53
1:2:594:GLN:HE22	1:2:651:ASN:HD21	1.55	0.53
1:2:574:TYR:HE1	2:2:931:HOH:O	1.91	0.53
1:1:471:MET:SD	1:1:471:MET:C	2.86	0.53
1:2:723:LEU:O	1:2:753:ILE:HG21	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:594:GLN:HE22	1:2:651:ASN:ND2	2.07	0.53
1:2:527:ASP:C	1:2:529:GLU:N	2.60	0.53
1:1:409:HIS:HE1	2:1:1174:HOH:O	1.92	0.52
1:2:430:MET:HE1	1:2:491:VAL:HG13	1.90	0.52
1:1:527:ASP:CB	1:1:528:PRO:HD2	2.40	0.52
1:1:442:PHE:O	1:1:446:LEU:HB2	2.09	0.52
1:1:573:VAL:O	1:1:576:LYS:HE2	2.09	0.52
1:1:518:ILE:HG22	1:1:518:ILE:O	2.08	0.52
1:2:546:ILE:HG22	1:2:550:ASN:ND2	2.25	0.52
1:2:620:TRP:HD1	1:2:625:GLN:HG3	1.75	0.51
1:2:637:LEU:HD12	1:2:699:VAL:HG21	1.91	0.51
1:2:413:LYS:HB3	1:2:414:GLU:OE1	2.11	0.51
1:2:732:LEU:HD11	2:2:905:HOH:O	2.10	0.51
1:1:482:THR:HG23	1:1:484:GLN:HG2	1.92	0.51
1:1:588:GLY:O	1:1:592:VAL:HG23	2.11	0.51
1:1:527:ASP:HB3	1:1:528:PRO:HD2	1.93	0.51
1:2:794:LEU:HD23	1:2:794:LEU:N	2.23	0.51
1:2:514:ILE:HD13	1:2:599:GLY:CA	2.41	0.51
1:1:641:LYS:HE3	2:1:916:HOH:O	2.10	0.51
1:2:693:TYR:HA	1:2:714:PHE:CE1	2.33	0.50
1:2:771:GLN:HB2	2:2:905:HOH:O	2.11	0.50
1:1:543:GLU:CD	1:1:543:GLU:H	2.14	0.50
1:2:541:LEU:HD23	1:2:541:LEU:O	2.11	0.50
1:2:441:GLU:HG2	1:2:506:TRP:CZ2	2.45	0.50
1:2:761:SER:OG	1:2:764:GLU:HG3	2.11	0.50
1:2:682:LEU:O	1:2:686:LYS:HG3	2.11	0.50
1:1:786:ASN:N	2:1:1156:HOH:O	2.45	0.50
1:2:783:MET:C	1:2:785:ALA:H	2.14	0.50
1:1:695:LEU:O	1:1:699:VAL:HG23	2.12	0.50
1:2:610:LYS:NZ	1:2:610:LYS:HB3	2.27	0.49
1:2:637:LEU:HD13	1:2:699:VAL:HG11	1.94	0.49
1:1:620:TRP:HD1	1:1:625:GLN:HG3	1.77	0.49
1:1:450:THR:OG1	1:1:451:PRO:HD2	2.13	0.49
1:2:548:VAL:O	1:2:552:GLN:HG2	2.13	0.49
1:1:754:LEU:O	1:1:757:ARG:HB2	2.13	0.49
1:2:448:ARG:HG3	1:2:448:ARG:NH1	2.28	0.49
1:2:641:LYS:N	1:2:642:PRO:HD2	2.28	0.49
1:2:771:GLN:HG3	2:2:826:HOH:O	2.12	0.48
1:2:731:ILE:HD11	1:2:768:ILE:CG2	2.43	0.48
1:2:430:MET:HA	1:2:471:MET:HE1	1.93	0.48
1:2:445:PHE:CE2	1:2:513:GLU:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:482:THR:CG2	1:1:484:GLN:HG2	2.42	0.48
1:2:463:ASP:O	1:2:466:LYS:N	2.45	0.48
1:2:655:ASN:O	1:2:659:GLU:HB2	2.13	0.48
1:2:751:VAL:O	1:2:755:LYS:HG3	2.13	0.48
1:1:774:GLU:HG3	2:1:1111:HOH:O	2.12	0.48
1:1:607:ASP:OD2	1:1:636:TYR:OH	2.29	0.48
1:2:739:LEU:CD2	1:2:776:LEU:HA	2.43	0.48
1:2:794:LEU:CD2	1:2:794:LEU:H	2.26	0.48
1:1:682:LEU:HD22	1:1:686:LYS:HE2	1.94	0.48
1:1:527:ASP:CB	1:1:528:PRO:CD	2.92	0.48
1:2:731:ILE:HD11	1:2:768:ILE:HG21	1.95	0.47
1:2:540:GLY:HA2	2:2:924:HOH:O	2.13	0.47
1:1:743:TRP:CE3	1:1:783:MET:HE1	2.49	0.47
1:2:615:ILE:HD13	1:2:667:ALA:CB	2.44	0.47
1:1:675:LYS:HG3	2:1:1200:HOH:O	2.13	0.47
1:1:785:ALA:HB3	2:1:1156:HOH:O	2.14	0.47
1:2:635:GLU:HB3	2:2:865:HOH:O	2.15	0.47
1:1:526:ILE:O	1:1:527:ASP:O	2.33	0.46
1:2:447:GLU:O	1:2:449:SER:N	2.45	0.46
1:2:661:ILE:HG23	1:2:717:MET:CE	2.46	0.46
1:1:502:ARG:HD2	2:1:818:HOH:O	2.15	0.46
1:2:472:PHE:HE2	1:2:562:ILE:HD13	1.79	0.46
1:1:518:ILE:CG2	1:1:518:ILE:O	2.63	0.46
1:2:407:GLY:HA2	2:2:849:HOH:O	2.15	0.46
1:2:448:ARG:HH11	1:2:448:ARG:HG3	1.80	0.46
1:2:437:LEU:HD21	1:2:468:CYS:HB2	1.98	0.46
1:2:448:ARG:HD2	1:2:539:GLY:O	2.16	0.46
1:1:441:GLU:HG2	1:1:506:TRP:CZ2	2.48	0.46
1:2:652:PHE:HZ	2:2:842:HOH:O	1.99	0.45
1:1:460:LEU:HG	1:1:643:GLN:HB3	1.98	0.45
1:2:616:PHE:CE2	1:2:685:MET:CE	2.88	0.45
1:2:601:ILE:N	2:2:842:HOH:O	2.49	0.45
1:2:766:LYS:NZ	2:2:938:HOH:O	2.44	0.45
1:1:540:GLY:HA2	1:1:543:GLU:OE1	2.16	0.45
1:2:450:THR:OG1	1:2:451:PRO:HD2	2.17	0.45
1:1:625:GLN:HE21	1:1:625:GLN:HB3	1.47	0.45
1:1:644:MET:CE	1:1:649:PHE:CA	2.88	0.44
1:1:780:ARG:HA	1:1:783:MET:HE2	2.00	0.44
1:1:510:ILE:HD11	1:1:548:VAL:HG11	1.98	0.44
1:2:501:LYS:CD	1:2:505:ASN:HD21	2.30	0.44
1:1:542:VAL:HG13	1:1:600:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:645:ASN:HD22	1:2:648:LEU:H	1.66	0.44
1:1:552:GLN:NE2	1:1:589:PHE:HD2	2.16	0.43
1:2:477:GLU:OE1	1:2:477:GLU:HA	2.18	0.43
1:1:412:ASP:O	1:1:416:GLU:HG2	2.18	0.43
1:1:615:ILE:O	1:1:616:PHE:HB2	2.18	0.43
1:2:616:PHE:O	1:2:672:HIS:CD2	2.72	0.43
1:1:423:LEU:HG	1:1:487:ILE:HA	2.00	0.43
1:1:556:ALA:O	1:1:560:VAL:HG23	2.19	0.43
1:2:667:ALA:C	1:2:669:SER:H	2.22	0.42
1:1:528:PRO:HG3	2:1:1007:HOH:O	2.19	0.42
1:2:739:LEU:HD21	1:2:776:LEU:CD1	2.49	0.42
1:2:441:GLU:CG	1:2:506:TRP:HZ2	2.32	0.42
1:2:747:ILE:HG22	2:2:893:HOH:O	2.18	0.42
1:2:448:ARG:HH21	1:2:541:LEU:HG	1.85	0.42
1:1:675:LYS:CB	1:1:680:LYS:HE3	2.44	0.42
1:2:472:PHE:CE2	1:2:476:VAL:HG11	2.54	0.42
1:2:567:GLY:CA	1:2:575:GLU:HG3	2.50	0.42
1:2:562:ILE:HD11	2:2:946:HOH:O	2.20	0.42
1:2:463:ASP:O	1:2:464:GLY:C	2.56	0.42
1:1:482:THR:CG2	1:1:484:GLN:HB2	2.50	0.41
1:2:617:SER:HB2	2:2:861:HOH:O	2.19	0.41
1:2:460:LEU:HG	1:2:643:GLN:HB3	2.01	0.41
1:2:615:ILE:HD11	1:2:616:PHE:CZ	2.55	0.41
1:1:651:ASN:ND2	2:1:841:HOH:O	2.52	0.41
1:2:694:GLN:HE21	1:2:694:GLN:CA	2.21	0.41
1:2:653:ILE:O	1:2:657:ILE:HG13	2.20	0.41
1:2:503:GLN:OE1	1:2:588:GLY:HA3	2.20	0.41
1:1:427:VAL:CG1	1:1:494:ARG:NH1	2.78	0.41
1:1:495:PHE:O	1:1:499:LEU:HG	2.21	0.41
1:2:546:ILE:O	1:2:550:ASN:ND2	2.54	0.41
1:1:616:PHE:HA	1:1:620:TRP:CE3	2.56	0.41
1:1:610:LYS:N	1:1:611:PRO:HD2	2.36	0.41
1:2:757:ARG:NH1	1:2:759:ASP:OD1	2.54	0.41
1:1:641:LYS:HB3	1:1:642:PRO:HD3	2.02	0.41
1:2:610:LYS:HB3	1:2:611:PRO:CD	2.51	0.41
1:2:694:GLN:NE2	1:2:694:GLN:CA	2.82	0.41
1:2:455:ASP:HB3	1:2:461:PHE:CE2	2.55	0.41
1:2:674:PHE:HE2	2:2:837:HOH:O	2.04	0.41
1:1:527:ASP:C	1:1:529:GLU:H	2.24	0.40
1:2:437:LEU:O	1:2:441:GLU:HB2	2.21	0.40
1:1:462:LEU:HD13	2:1:843:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:426:ILE:O	1:2:429:LYS:HB3	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:806:HOH:O	2:1:851:HOH:O[2_555]	1.96	0.24
2:1:817:HOH:O	2:1:848:HOH:O[2_545]	2.12	0.08

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	1	397/399 (100%)	379 (96%)	16 (4%)	2 (0%)	34	48
1	2	392/399 (98%)	353 (90%)	34 (9%)	5 (1%)	15	21
All	All	789/798 (99%)	732 (93%)	50 (6%)	7 (1%)	21	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	527	ASP
1	1	528	PRO
1	2	528	PRO
1	2	530	SER
1	2	527	ASP
1	2	804	LYS
1	2	704	GLU

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	1	348/364 (96%)	322 (92%)	26 (8%)	17	26
1	2	324/364 (89%)	305 (94%)	19 (6%)	24	38
All	All	672/728 (92%)	627 (93%)	45 (7%)	20	31

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	418	LEU
1	1	423	LEU
1	1	427	VAL
1	1	446	LEU
1	1	457	ASP
1	1	476	VAL
1	1	482	THR
1	1	483	ASN
1	1	488	LEU
1	1	522	HIS
1	1	527	ASP
1	1	528	PRO
1	1	529	GLU
1	1	531	ILE
1	1	541	LEU
1	1	543	GLU
1	1	600	LEU
1	1	625	GLN
1	1	643	GLN
1	1	665	LEU
1	1	682	LEU
1	1	704	GLU
1	1	709	LEU
1	1	750	LEU
1	1	794	LEU
1	1	796	ARG
1	2	414	GLU

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Mol	Chain	Res	Type
1	2	418	LEU
1	2	421	ASP
1	2	423	LEU
1	2	427	VAL
1	2	432	GLU
1	2	446	LEU
1	2	471	MET
1	2	477	GLU
1	2	541	LEU
1	2	557	ASP
1	2	615	ILE
1	2	625	GLN
1	2	662	ILE
1	2	665	LEU
1	2	731	ILE
1	2	750	LEU
1	2	763	SER
1	2	770	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	474	GLN
1	1	475	GLN
1	1	483	ASN
1	1	552	GLN
1	1	577	GLN
1	1	581	HIS
1	1	613	GLN
1	1	625	GLN
1	1	645	ASN
1	1	651	ASN
1	2	470	GLN
1	2	475	GLN
1	2	505	ASN
1	2	577	GLN
1	2	625	GLN
1	2	643	GLN
1	2	645	ASN
1	2	651	ASN
1	2	672	HIS
1	2	694	GLN

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Mol	Chain	Res	Type
1	2	712	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1	399/399 (100%)	-0.08	6 (1%) 76 75	32, 53, 84, 141	28 (7%)
1	2	396/399 (99%)	-0.10	6 (1%) 76 75	49, 77, 112, 164	46 (11%)
All	All	795/798 (99%)	-0.09	12 (1%) 76 75	32, 66, 109, 164	74 (9%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	529	GLU	5.0
1	2	531	ILE	3.4
1	1	529	GLU	3.3
1	1	530	SER	3.0
1	2	530	SER	3.0
1	1	528	PRO	2.8
1	1	534	GLU	2.5
1	2	674	PHE	2.3
1	1	531	ILE	2.2
1	2	743	TRP	2.2
1	1	527	ASP	2.2
1	2	741	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.