



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:35 PM GMT

PDB ID : 3U82
Title : Binding of herpes simplex virus glycoprotein D to nectin-1 exploits host cell adhesion
Authors : Zhang, N.; Yan, J.; Lu, G.; Guo, Z.; Fan, Z.; Wang, J.; Shi, Y.; Qi, J.; Gao, G.F.
Deposited on : 2011-10-15
Resolution : 3.16 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

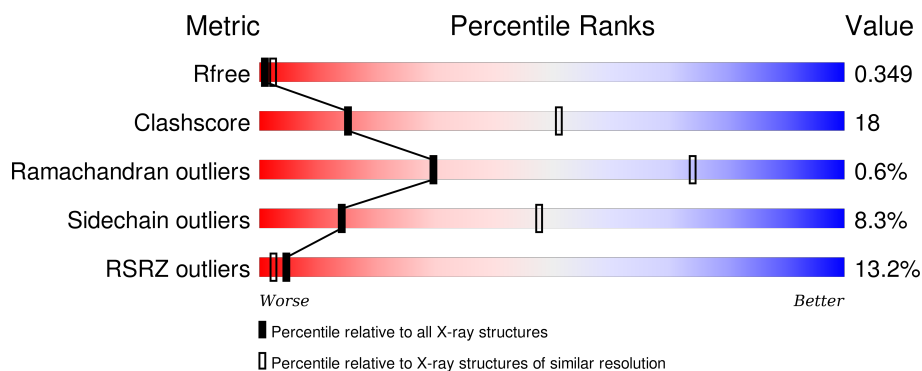
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	A	291	<div> <div>6%</div> <div>66%</div> <div>12%</div> <div>•</div> <div>21%</div> </div>
2	B	317	<div> <div>16%</div> <div>69%</div> <div>20%</div> <div>6%</div> <div>5%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4178 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 Envelope glycoprotein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	231	1818	1167	311	330	10	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	HIS	-	EXPRESSION TAG	UNP Q69091
A	287	HIS	-	EXPRESSION TAG	UNP Q69091
A	288	HIS	-	EXPRESSION TAG	UNP Q69091
A	289	HIS	-	EXPRESSION TAG	UNP Q69091
A	290	HIS	-	EXPRESSION TAG	UNP Q69091
A	291	HIS	-	EXPRESSION TAG	UNP Q69091

- Molecule 2 is a protein called Poliovirus receptor-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	300	2360	1483	409	457	11	0	1	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	336	ALA	-	EXPRESSION TAG	UNP Q15223
B	337	ALA	-	EXPRESSION TAG	UNP Q15223
B	338	ALA	-	EXPRESSION TAG	UNP Q15223
B	339	LEU	-	EXPRESSION TAG	UNP Q15223
B	340	GLU	-	EXPRESSION TAG	UNP Q15223
B	341	HIS	-	EXPRESSION TAG	UNP Q15223
B	342	HIS	-	EXPRESSION TAG	UNP Q15223
B	343	HIS	-	EXPRESSION TAG	UNP Q15223
B	344	HIS	-	EXPRESSION TAG	UNP Q15223
B	345	HIS	-	EXPRESSION TAG	UNP Q15223

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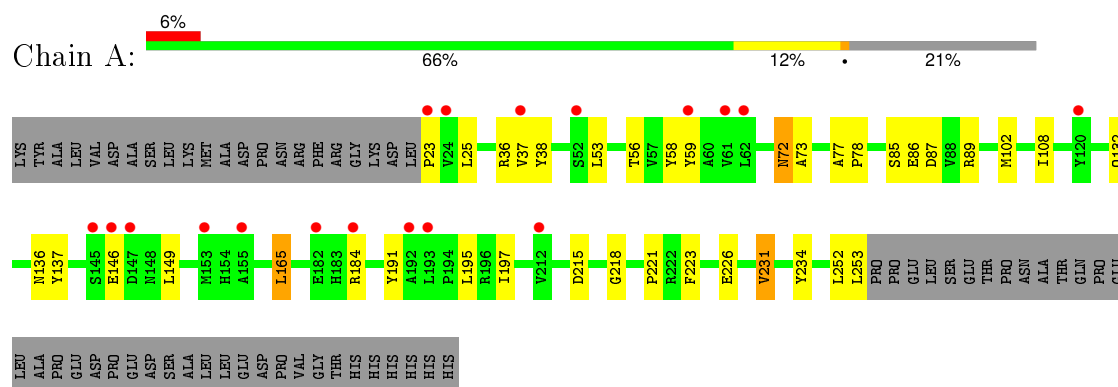
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Chain	Residue	Modelled	Actual	Comment	Reference
B	346	HIS	-	EXPRESSION TAG	UNP Q15223

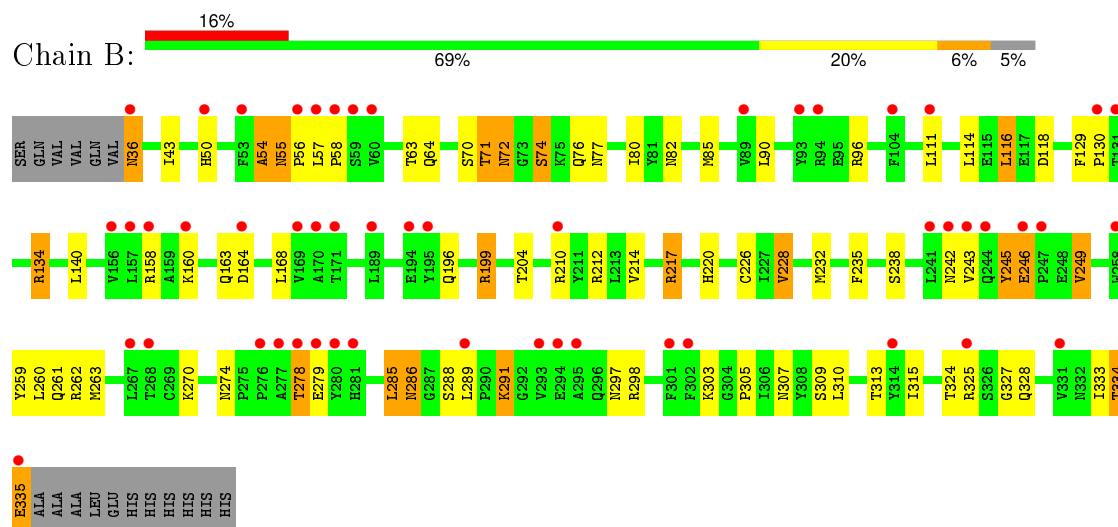
3 Residue-property plots [i](#)

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: Envelope glycoprotein D



• Molecule 2: Poliovirus receptor-related protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	52.53Å 169.04Å 183.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.38 – 3.16 38.38 – 3.16	Depositor EDS
% Data completeness (in resolution range)	81.9 (38.38-3.16) 94.1 (38.38-3.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.321 , 0.344 0.322 , 0.349	Depositor DCC
R_{free} test set	671 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	105.3	Xtriage
Anisotropy	0.843	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 121.6	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	1 of 13551 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4178	wwPDB-VP
Average B, all atoms (Å ²)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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	A	0.57	0/1877	0.78	1/2567 (0.0%)
2	B	0.31	0/2413	0.56	3/3287 (0.1%)
All	All	0.44	0/4290	0.67	4/5854 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	246	GLU	N-CA-CB	-8.04	96.13	110.60
2	B	246	GLU	N-CA-C	7.34	130.81	111.00
2	B	72	ASN	N-CA-C	5.95	127.05	111.00
1	A	87	ASP	CB-CG-OD2	5.55	123.30	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	71	THR	Peptide

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	1818	0	1795	78	4
2	B	2360	0	2293	112	5
All	All	4178	0	4088	145	7

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 18.

All (145) 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:217:ARG:HD3	2:B:245:TYR:CE1	1.40	1.56
2:B:245:TYR:CE2	2:B:274:ASN:HB3	1.66	1.28
1:A:59:TYR:HE1	1:A:253:LEU:CB	1.50	1.23
2:B:217:ARG:CD	2:B:245:TYR:CE1	2.23	1.20
2:B:217:ARG:CD	2:B:245:TYR:HE1	1.55	1.20
2:B:245:TYR:HE2	2:B:274:ASN:CB	1.57	1.18
1:A:58:TYR:CE2	1:A:252:LEU:HB2	1.83	1.14
1:A:58:TYR:OH	1:A:252:LEU:HD12	1.45	1.13
1:A:221:PRO:HG2	2:B:64:GLN:NE2	1.64	1.11
1:A:223:PHE:CE2	2:B:63:THR:HG21	1.89	1.07
1:A:221:PRO:HG2	2:B:64:GLN:HE22	0.89	1.06
1:A:59:TYR:CE1	1:A:253:LEU:CB	2.39	1.04
2:B:245:TYR:HE2	2:B:274:ASN:HB3	0.87	1.01
1:A:218:GLY:HA2	2:B:77:ASN:ND2	1.78	0.98
1:A:58:TYR:CZ	1:A:252:LEU:HD12	1.98	0.97
1:A:58:TYR:OH	1:A:252:LEU:CD1	2.13	0.96
1:A:223:PHE:HE2	2:B:63:THR:HG1	1.09	0.93
1:A:132:GLN:NE2	2:B:85:MET:HE2	1.82	0.93
1:A:132:GLN:NE2	2:B:85:MET:CE	2.33	0.92
1:A:58:TYR:CZ	1:A:252:LEU:CD1	2.53	0.92
1:A:58:TYR:CE2	1:A:252:LEU:CB	2.53	0.91
1:A:221:PRO:CG	2:B:64:GLN:HE22	1.81	0.90
2:B:220:HIS:HD2	2:B:243:VAL:H	1.16	0.88
1:A:252:LEU:C	1:A:252:LEU:HD23	1.94	0.87
2:B:217:ARG:HB2	2:B:245:TYR:HD1	1.40	0.86
1:A:215:ASP:HB3	2:B:90:LEU:HD13	1.54	0.86
2:B:217:ARG:HD3	2:B:245:TYR:CD1	2.11	0.86
2:B:245:TYR:CD2	2:B:245:TYR:O	2.30	0.85
1:A:234:TYR:CZ	2:B:130:PRO:HB2	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:ALA:O	2:B:56:PRO:HD3	1.77	0.83
1:A:58:TYR:CZ	1:A:252:LEU:HG	2.13	0.81
2:B:220:HIS:CD2	2:B:243:VAL:H	1.98	0.81
2:B:245:TYR:CE2	2:B:274:ASN:CB	2.44	0.81
1:A:58:TYR:CE2	1:A:252:LEU:CG	2.64	0.81
2:B:297:ASN:HD22	2:B:298:ARG:H	1.27	0.80
1:A:252:LEU:CD2	1:A:252:LEU:O	2.30	0.80
1:A:58:TYR:CZ	1:A:252:LEU:CG	2.64	0.79
1:A:234:TYR:CE1	2:B:130:PRO:HB2	2.18	0.79
2:B:217:ARG:HB2	2:B:245:TYR:CD1	2.18	0.79
2:B:217:ARG:HD3	2:B:245:TYR:HE1	0.71	0.78
1:A:58:TYR:HE2	1:A:252:LEU:HB2	1.46	0.77
1:A:132:GLN:HE21	2:B:85:MET:CE	1.96	0.77
2:B:220:HIS:CE1	2:B:274:ASN:OD1	2.38	0.76
1:A:215:ASP:CB	2:B:90:LEU:HD13	2.15	0.76
1:A:223:PHE:CE2	2:B:63:THR:CG2	2.69	0.73
2:B:199:ARG:HH11	2:B:199:ARG:HG3	1.52	0.73
2:B:307:ASN:HD22	2:B:309:SER:H	1.38	0.71
1:A:252:LEU:CD2	1:A:252:LEU:C	2.60	0.70
2:B:36:ASN:HD22	2:B:36:ASN:N	1.90	0.69
2:B:70:SER:HA	2:B:74:SER:O	1.93	0.69
2:B:134:ARG:HG3	2:B:134:ARG:HH11	1.59	0.68
2:B:249:VAL:HG22	2:B:327:GLY:HA3	1.76	0.67
1:A:36:ARG:HB2	2:B:85:MET:SD	2.35	0.67
1:A:36:ARG:C	2:B:85:MET:HE3	2.15	0.67
1:A:218:GLY:CA	2:B:77:ASN:ND2	2.57	0.66
1:A:252:LEU:O	1:A:253:LEU:C	2.30	0.66
1:A:215:ASP:CG	2:B:90:LEU:HD13	2.16	0.65
1:A:218:GLY:HA2	2:B:77:ASN:HD21	1.58	0.65
2:B:286:ASN:ND2	2:B:286:ASN:O	2.30	0.65
2:B:199:ARG:HH11	2:B:199:ARG:CG	2.09	0.65
1:A:58:TYR:CE2	1:A:252:LEU:HD12	2.32	0.64
2:B:307:ASN:O	2:B:333:ILE:HD13	1.97	0.64
2:B:245:TYR:CE2	2:B:274:ASN:N	2.65	0.64
1:A:252:LEU:O	1:A:252:LEU:HD23	1.93	0.64
1:A:252:LEU:O	1:A:252:LEU:HD22	1.97	0.63
1:A:72:ASN:HD22	1:A:73:ALA:H	1.44	0.63
1:A:58:TYR:CE2	1:A:252:LEU:HG	2.33	0.62
1:A:36:ARG:O	2:B:85:MET:HE3	1.99	0.62
2:B:134:ARG:NH1	2:B:134:ARG:HG3	2.13	0.61
2:B:245:TYR:HE2	2:B:274:ASN:CA	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:LEU:HD21	2:B:204:THR:HG23	1.82	0.61
2:B:286:ASN:HD22	2:B:286:ASN:C	2.04	0.60
1:A:215:ASP:CG	2:B:90:LEU:CD1	2.70	0.60
2:B:228:VAL:HG13	2:B:235:PHE:HB3	1.84	0.60
1:A:218:GLY:CA	2:B:77:ASN:HD21	2.15	0.59
2:B:310:LEU:HB2	2:B:333:ILE:HD11	1.84	0.59
2:B:297:ASN:ND2	2:B:298:ARG:H	2.00	0.58
1:A:23:PRO:O	2:B:130:PRO:HG3	2.03	0.58
1:A:223:PHE:HE2	2:B:63:THR:HG21	1.64	0.58
1:A:23:PRO:O	2:B:130:PRO:CG	2.51	0.58
2:B:217:ARG:HD2	2:B:245:TYR:CE1	2.32	0.58
1:A:36:ARG:HB3	2:B:85:MET:HE1	1.87	0.57
1:A:218:GLY:C	2:B:77:ASN:HD21	2.09	0.56
1:A:25:LEU:HB2	2:B:129:PHE:HE2	1.71	0.55
2:B:260:LEU:O	2:B:261:GLN:HB2	2.06	0.55
2:B:134:ARG:CG	2:B:134:ARG:HH11	2.20	0.54
2:B:249:VAL:CG2	2:B:327:GLY:HA3	2.37	0.54
1:A:58:TYR:CD2	1:A:252:LEU:HB2	2.40	0.54
1:A:223:PHE:HE2	2:B:63:THR:CG2	2.17	0.53
1:A:23:PRO:HB3	2:B:130:PRO:HG2	1.91	0.53
1:A:223:PHE:HE2	2:B:63:THR:OG1	1.85	0.52
2:B:334:THR:HG23	2:B:335:GLU:N	2.25	0.52
2:B:196:GLN:OE1	2:B:210:ARG:NH2	2.39	0.52
2:B:43:ILE:HD11	2:B:116:LEU:HD13	1.91	0.51
2:B:262:ARG:HG3	2:B:263:MET:N	2.24	0.51
1:A:36:ARG:C	2:B:85:MET:CE	2.79	0.51
2:B:297:ASN:HD22	2:B:298:ARG:N	2.02	0.50
2:B:324:THR:O	2:B:325:ARG:HD2	2.12	0.50
1:A:58:TYR:CE2	1:A:252:LEU:CD1	2.90	0.50
1:A:85:SER:O	1:A:89:ARG:HG3	2.11	0.50
2:B:307:ASN:ND2	2:B:309:SER:H	2.05	0.50
2:B:71:THR:HG23	2:B:71:THR:O	2.12	0.50
1:A:58:TYR:CE1	1:A:252:LEU:HG	2.47	0.49
2:B:71:THR:HG22	2:B:74:SER:OG	2.13	0.49
1:A:223:PHE:CD2	2:B:63:THR:HG21	2.45	0.49
1:A:25:LEU:HB2	2:B:129:PHE:CE2	2.48	0.49
2:B:199:ARG:NH1	2:B:199:ARG:CG	2.71	0.48
2:B:245:TYR:CG	2:B:245:TYR:O	2.65	0.48
2:B:261:GLN:HA	2:B:305:PRO:HB2	1.96	0.48
2:B:278:THR:HG22	2:B:279:GLU:HB2	1.96	0.47
1:A:231:VAL:HG12	2:B:129:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:TYR:CD2	1:A:252:LEU:CB	2.97	0.46
1:A:23:PRO:O	2:B:130:PRO:HG2	2.15	0.46
2:B:285:LEU:HD13	2:B:285:LEU:HA	1.66	0.46
1:A:234:TYR:OH	2:B:130:PRO:HB2	2.16	0.45
2:B:286:ASN:ND2	2:B:286:ASN:C	2.68	0.45
2:B:160:LYS:O	2:B:163:GLN:HB2	2.16	0.45
1:A:231:VAL:HG12	2:B:129:PHE:HE1	1.82	0.45
2:B:291:LYS:HB3	2:B:291:LYS:HE2	1.88	0.45
1:A:136:ASN:HB3	1:A:137:TYR:CD1	2.52	0.45
1:A:36:ARG:CB	2:B:85:MET:CE	2.95	0.44
1:A:108:ILE:HD13	1:A:197:ILE:HG21	1.99	0.44
2:B:57:LEU:HB3	2:B:58:PRO:HD2	2.00	0.44
2:B:80:ILE:N	2:B:80:ILE:HD12	2.33	0.44
1:A:77:ALA:HB3	1:A:78:PRO:HD3	2.01	0.43
1:A:58:TYR:OH	1:A:252:LEU:HD11	2.12	0.43
1:A:132:GLN:NE2	2:B:85:MET:HE1	2.26	0.43
1:A:56:THR:HG1	1:A:58:TYR:HE1	1.66	0.43
2:B:217:ARG:CD	2:B:245:TYR:CD1	2.88	0.42
2:B:57:LEU:N	2:B:57:LEU:HD12	2.33	0.42
1:A:38:TYR:OH	2:B:82:ASN:CB	2.67	0.42
1:A:38:TYR:OH	2:B:82:ASN:HB2	2.18	0.42
2:B:96:ARG:NH2	2:B:118:ASP:OD2	2.49	0.42
1:A:102:MET:SD	1:A:165:LEU:HD22	2.60	0.42
1:A:25:LEU:CB	2:B:129:PHE:HE2	2.33	0.42
2:B:245:TYR:CE2	2:B:274:ASN:CA	2.96	0.41
1:A:132:GLN:HE22	2:B:85:MET:HE2	1.75	0.41
2:B:168:LEU:HA	2:B:212:ARG:HG2	2.03	0.41
2:B:259:TYR:CE2	2:B:262:ARG:HB2	2.56	0.41
2:B:315:ILE:HG12	2:B:328:GLN:HG2	2.03	0.41
1:A:36:ARG:CB	2:B:85:MET:SD	3.07	0.41
2:B:249:VAL:HG22	2:B:327:GLY:CA	2.49	0.41
2:B:285:LEU:HD23	2:B:313:THR:HG21	2.02	0.41
2:B:55:ASN:O	2:B:57:LEU:HD12	2.21	0.41

All (7) 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:B:50[B]:HIS:NE2	2:B:335:GLU:CG[7_654]	1.76	0.44
1:A:191:TYR:OH	2:B:158:ARG:NH2[5_455]	1.84	0.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:OE1	1:A:146:GLU:OE2[4_555]	1.99	0.21
2:B:50[B]:HIS:CE1	2:B:335:GLU:OE2[7_654]	2.04	0.16
2:B:50[B]:HIS:NE2	2:B:335:GLU:CD[7_654]	2.09	0.11
1:A:146:GLU:OE1	1:A:146:GLU:OE1[4_555]	2.16	0.04
1:A:85:SER:CB	2:B:238:SER:O[8_445]	2.18	0.02

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	230/291 (79%)	224 (97%)	6 (3%)	0	100	100
2	B	299/317 (94%)	283 (95%)	13 (4%)	3 (1%)	19	63
All	All	529/608 (87%)	507 (96%)	19 (4%)	3 (1%)	30	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	ALA
2	B	72	ASN
2	B	246	GLU

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	198/250 (79%)	189 (96%)	9 (4%)	34	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	261/276 (95%)	232 (89%)	29 (11%)	8	31
All	All	459/526 (87%)	421 (92%)	38 (8%)	14	48

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	53	LEU
1	A	72	ASN
1	A	86	GLU
1	A	149	LEU
1	A	165	LEU
1	A	184	ARG
1	A	195	LEU
1	A	231	VAL
2	B	36	ASN
2	B	55	ASN
2	B	74	SER
2	B	76	GLN
2	B	111	LEU
2	B	114	LEU
2	B	116	LEU
2	B	134	ARG
2	B	140	LEU
2	B	164	ASP
2	B	199	ARG
2	B	214	VAL
2	B	217	ARG
2	B	226	CYS
2	B	228	VAL
2	B	232	MET
2	B	242	ASN
2	B	245	TYR
2	B	249	VAL
2	B	270	LYS
2	B	278	THR
2	B	285	LEU
2	B	286	ASN
2	B	288	SER
2	B	289	LEU
2	B	291	LYS
2	B	303	LYS

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Mol	Chain	Res	Type
2	B	334	THR
2	B	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	72	ASN
1	A	132	GLN
2	B	72	ASN
2	B	76	GLN
2	B	77	ASN
2	B	163	GLN
2	B	220	HIS
2	B	281	HIS
2	B	286	ASN
2	B	296	GLN
2	B	297	ASN
2	B	307	ASN

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/291 (79%)	0.73	18 (7%) 16 8	98, 169, 268, 369	0
2	B	300/317 (94%)	0.84	52 (17%) 2 1	108, 194, 321, 503	0
All	All	531/608 (87%)	0.80	70 (13%) 4 2	98, 179, 291, 503	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	PRO	15.6
2	B	244	GLN	9.1
2	B	130	PRO	8.6
2	B	242	ASN	6.8
2	B	157	LEU	6.1
2	B	58	PRO	5.8
2	B	194	GLU	5.8
1	A	24	VAL	5.2
1	A	193	LEU	5.2
2	B	59	SER	4.8
2	B	56	PRO	4.7
2	B	247	PRO	4.5
2	B	60	VAL	4.5
2	B	335	GLU	4.3
2	B	267	LEU	4.3
2	B	170	ALA	4.2
2	B	276	PRO	4.2
2	B	156	VAL	4.1
2	B	277	ALA	4.0
2	B	243	VAL	4.0
2	B	289	LEU	3.9
2	B	293	VAL	3.9
2	B	53	PHE	3.8
1	A	120	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	153	MET	3.7
2	B	246	GLU	3.6
2	B	279	GLU	3.6
2	B	158	ARG	3.6
2	B	314	TYR	3.4
1	A	146	GLU	3.4
2	B	131	THR	3.3
1	A	61	VAL	3.3
2	B	160	LYS	3.3
2	B	281	HIS	3.3
1	A	192	ALA	3.2
1	A	184	ARG	3.0
2	B	189	LEU	3.0
2	B	195	TYR	3.0
2	B	302	PHE	3.0
2	B	280	TYR	2.9
2	B	241	LEU	2.6
2	B	164	ASP	2.6
2	B	331	VAL	2.6
1	A	59	TYR	2.6
2	B	111	LEU	2.5
2	B	268	THR	2.4
2	B	104	PHE	2.4
2	B	36	ASN	2.4
1	A	155	ALA	2.4
1	A	212	VAL	2.4
2	B	295	ALA	2.3
1	A	37	VAL	2.3
2	B	89	VAL	2.3
2	B	301	PHE	2.3
1	A	62	LEU	2.3
2	B	210	ARG	2.2
2	B	57	LEU	2.2
2	B	50[A]	HIS	2.2
2	B	258	TRP	2.2
1	A	182	GLU	2.2
2	B	169	VAL	2.2
1	A	52	SER	2.2
2	B	94	ARG	2.1
1	A	145	SER	2.1
2	B	325	ARG	2.1
2	B	93	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	147	ASP	2.0
2	B	171	THR	2.0
2	B	278	THR	2.0
2	B	294	GLU	2.0

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.