Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:08 PM GMT

PDB ID	:	3T1E
Title	:	The structure of the Newcastle disease virus hemagglutinin-neuraminidase (HN) ectodomain reveals a 4-helix bundle stalk
Authors	:	Yuan, P.; Swanson, K.; Leser, G.P.; Paterson, R.G.; Lamb, R.A.; Jardetzky, T.S.
Deposited on	:	2011-07-21
Resolution	:	3.30 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 (i) symbol.

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

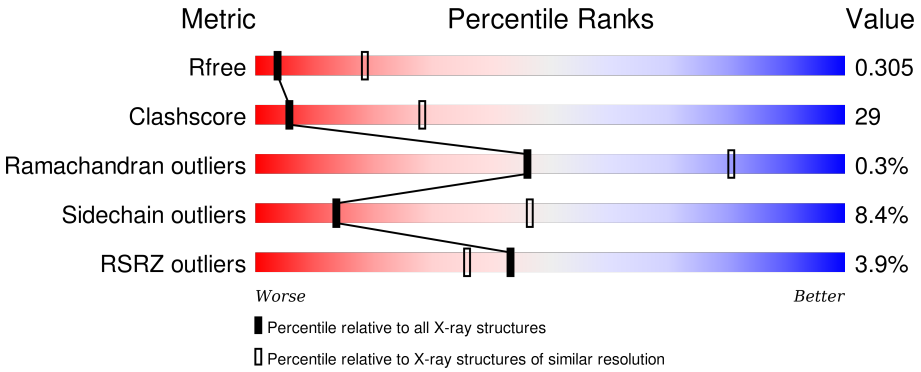
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	537	% 50% 31% · 17%
1	B	537	6% 48% 31% · 17%
1	E	537	· · · 93%
1	F	537	· · 93%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6976 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 Hemagglutinin-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3204	1989	549	646	20			
1	B	445	Total	C	N	O	S	0	0	0
			3194	1983	546	646	19			
1	E	37	Total	C	N	O	S	0	0	0
			289	184	46	58	1			
1	F	37	Total	C	N	O	S	0	0	0
			289	184	46	58	1			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ALA	-	EXPRESSION TAG	UNP P12554
A	35	MET	-	EXPRESSION TAG	UNP P12554
A	36	ALA	-	EXPRESSION TAG	UNP P12554
A	37	HIS	-	EXPRESSION TAG	UNP P12554
A	38	HIS	-	EXPRESSION TAG	UNP P12554
A	39	HIS	-	EXPRESSION TAG	UNP P12554
A	40	HIS	-	EXPRESSION TAG	UNP P12554
A	41	HIS	-	EXPRESSION TAG	UNP P12554
A	42	HIS	-	EXPRESSION TAG	UNP P12554
A	43	LEU	-	EXPRESSION TAG	UNP P12554
A	44	VAL	-	EXPRESSION TAG	UNP P12554
A	45	PRO	-	EXPRESSION TAG	UNP P12554
A	46	ARG	-	EXPRESSION TAG	UNP P12554
A	47	GLY	-	EXPRESSION TAG	UNP P12554
A	48	SER	-	EXPRESSION TAG	UNP P12554
A	328	ALA	GLY	SEE REMARK 999	UNP P12554
B	34	ALA	-	EXPRESSION TAG	UNP P12554
B	35	MET	-	EXPRESSION TAG	UNP P12554
B	36	ALA	-	EXPRESSION TAG	UNP P12554
B	37	HIS	-	EXPRESSION TAG	UNP P12554
B	38	HIS	-	EXPRESSION TAG	UNP P12554

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Chain	Residue	Modelled	Actual	Comment	Reference
B	39	HIS	-	EXPRESSION TAG	UNP P12554
B	40	HIS	-	EXPRESSION TAG	UNP P12554
B	41	HIS	-	EXPRESSION TAG	UNP P12554
B	42	HIS	-	EXPRESSION TAG	UNP P12554
B	43	LEU	-	EXPRESSION TAG	UNP P12554
B	44	VAL	-	EXPRESSION TAG	UNP P12554
B	45	PRO	-	EXPRESSION TAG	UNP P12554
B	46	ARG	-	EXPRESSION TAG	UNP P12554
B	47	GLY	-	EXPRESSION TAG	UNP P12554
B	48	SER	-	EXPRESSION TAG	UNP P12554
B	328	ALA	GLY	SEE REMARK 999	UNP P12554
E	34	ALA	-	EXPRESSION TAG	UNP P12554
E	35	MET	-	EXPRESSION TAG	UNP P12554
E	36	ALA	-	EXPRESSION TAG	UNP P12554
E	37	HIS	-	EXPRESSION TAG	UNP P12554
E	38	HIS	-	EXPRESSION TAG	UNP P12554
E	39	HIS	-	EXPRESSION TAG	UNP P12554
E	40	HIS	-	EXPRESSION TAG	UNP P12554
E	41	HIS	-	EXPRESSION TAG	UNP P12554
E	42	HIS	-	EXPRESSION TAG	UNP P12554
E	43	LEU	-	EXPRESSION TAG	UNP P12554
E	44	VAL	-	EXPRESSION TAG	UNP P12554
E	45	PRO	-	EXPRESSION TAG	UNP P12554
E	46	ARG	-	EXPRESSION TAG	UNP P12554
E	47	GLY	-	EXPRESSION TAG	UNP P12554
E	48	SER	-	EXPRESSION TAG	UNP P12554
E	328	ALA	GLY	SEE REMARK 999	UNP P12554
F	34	ALA	-	EXPRESSION TAG	UNP P12554
F	35	MET	-	EXPRESSION TAG	UNP P12554
F	36	ALA	-	EXPRESSION TAG	UNP P12554
F	37	HIS	-	EXPRESSION TAG	UNP P12554
F	38	HIS	-	EXPRESSION TAG	UNP P12554
F	39	HIS	-	EXPRESSION TAG	UNP P12554
F	40	HIS	-	EXPRESSION TAG	UNP P12554
F	41	HIS	-	EXPRESSION TAG	UNP P12554
F	42	HIS	-	EXPRESSION TAG	UNP P12554
F	43	LEU	-	EXPRESSION TAG	UNP P12554
F	44	VAL	-	EXPRESSION TAG	UNP P12554
F	45	PRO	-	EXPRESSION TAG	UNP P12554
F	46	ARG	-	EXPRESSION TAG	UNP P12554
F	47	GLY	-	EXPRESSION TAG	UNP P12554
F	48	SER	-	EXPRESSION TAG	UNP P12554

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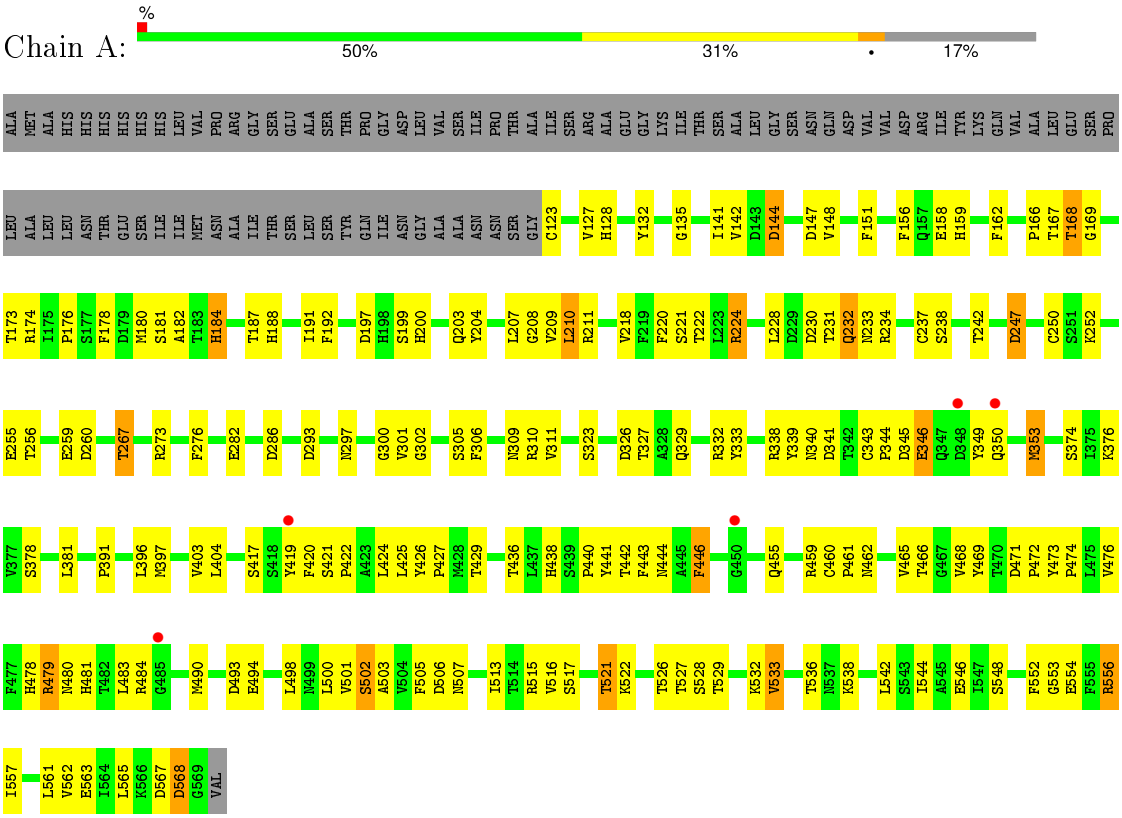
Chain	Residue	Modelled	Actual	Comment	Reference
F	328	ALA	GLY	SEE REMARK 999	UNP P12554

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.

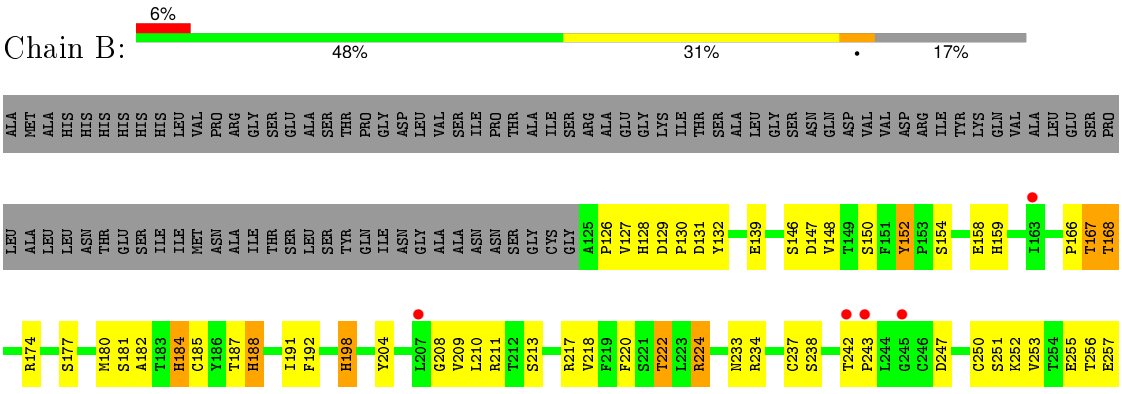
- Molecule 1: Hemagglutinin-neuraminidase

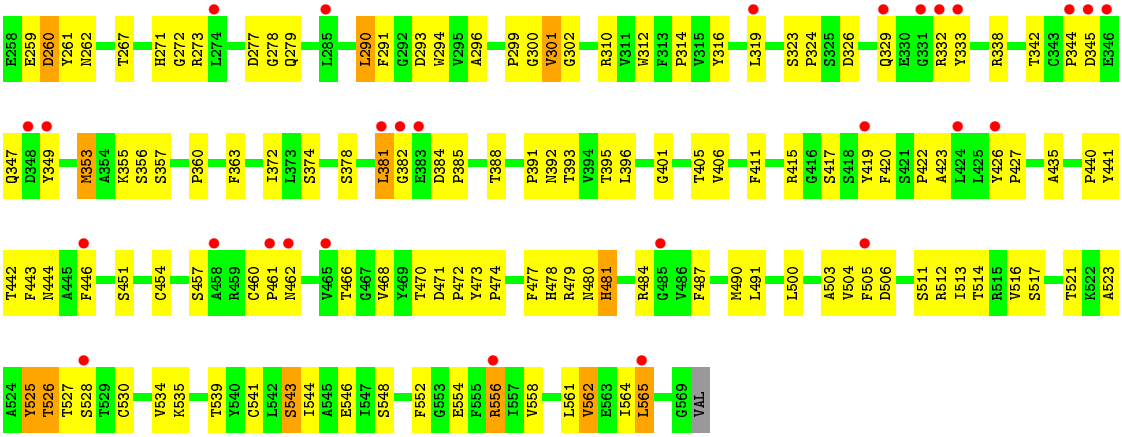
Chain A:



- Molecule 1: Hemagglutinin-neuraminidase

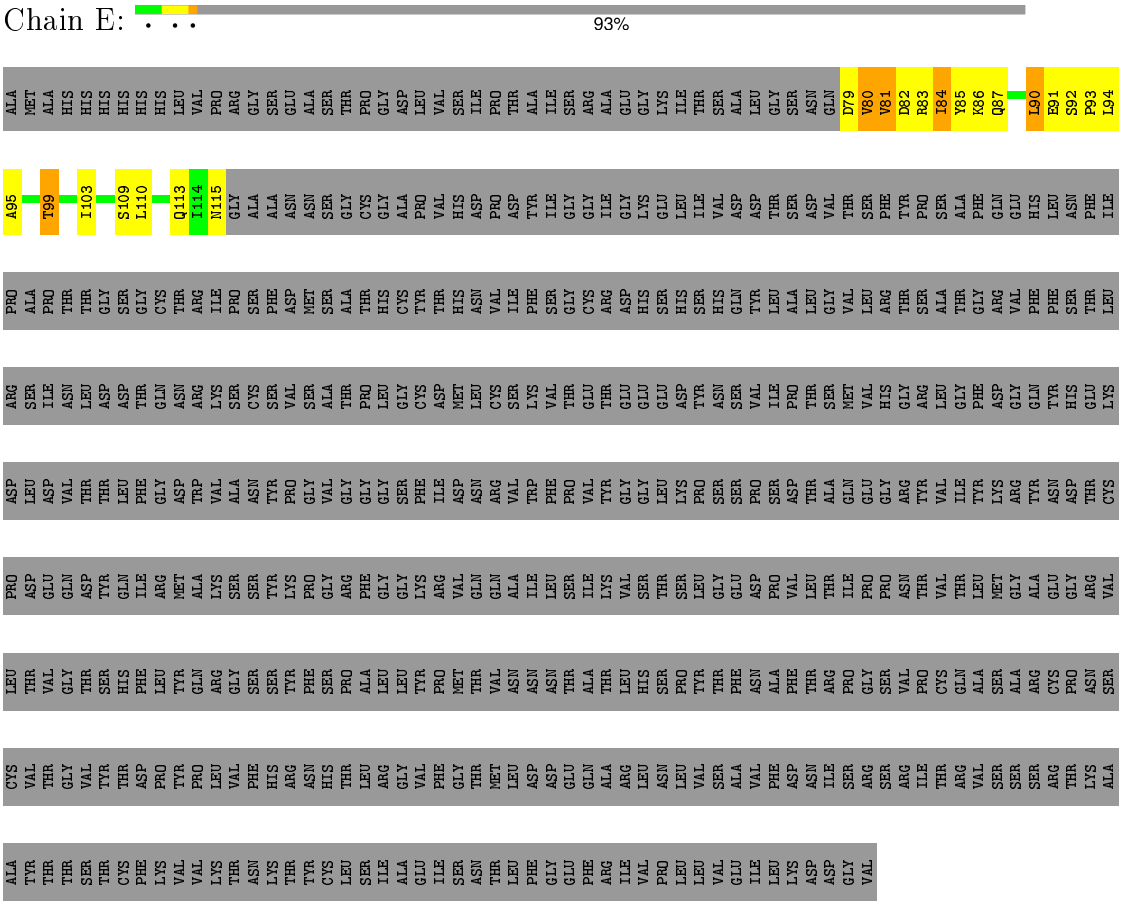
Chain B:





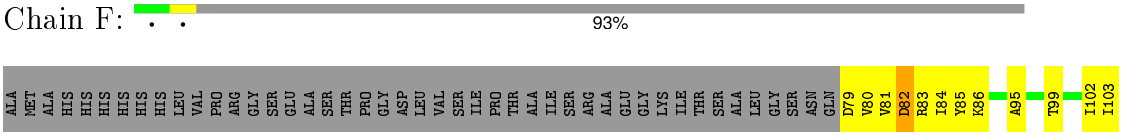
- Molecule 1: Hemagglutinin-neuraminidase

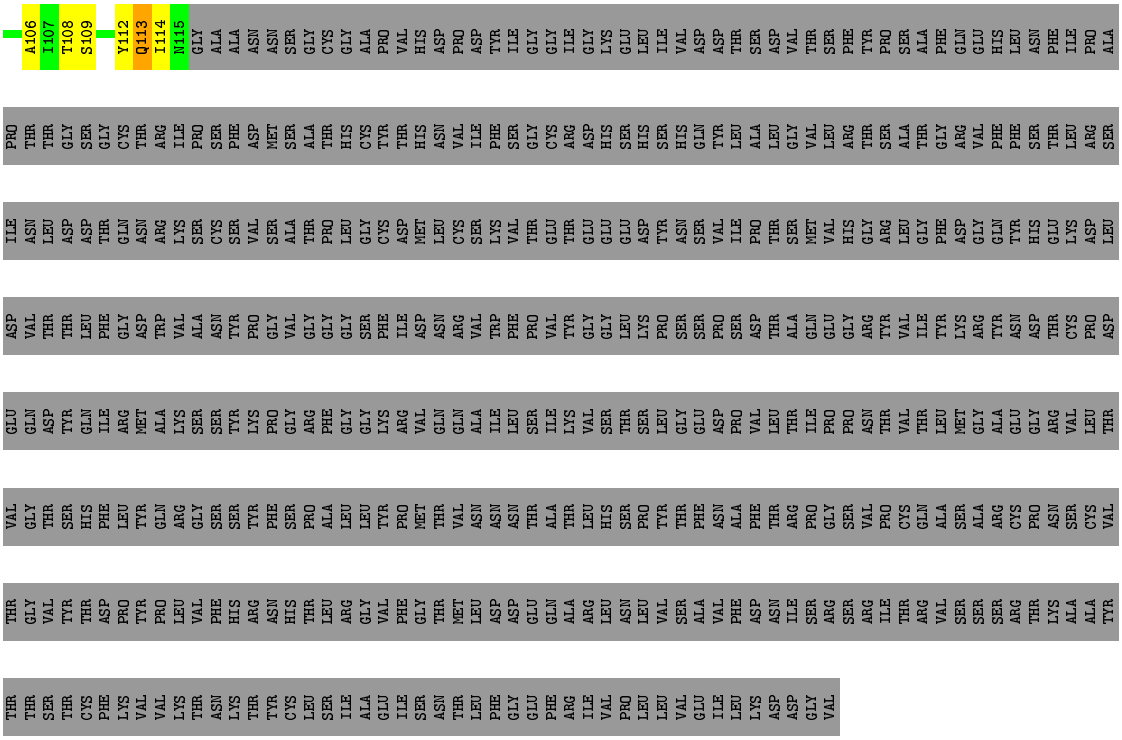
Chain E:



- Molecule 1: Hemagglutinin-neuraminidase

Chain F:




A106 T107 T108 S109 Y112 Q113 I114 N115
GLY ALA ALA ASN ASN SER GLY CYS GLY ALA PRO VAL HIS ASP PRO ASP TYR ILE GLY GLY ILE GLY LYS GLU LEU ILE VAL ASP ASP THR SER ASP VAL THR SER PHE TYR PRO SER ALA PHE GLN GLU HIS LEU ASN PHE ILE PRO ALA
PRO THR THR GLY SER GLY CYS THR ARG ILE PRO SER PHE ASP MET SER ALA THR HIS CYS TYR THR HIS ASN VAL ILE PHE SER GLY CYS ARG ASP HIS SER HIS SER HIS GLN TYR LEU ALA LEU GLY VAL LEU ARG THR SER ALA THR GLY ARG VAL PHE PHE SER THR LEU ARG SER
ILE ASN LEU ASP ASP THR GLN ASN ARG LYS SER CYS SER VAL SER ALA THR PRO LEU GLY CYS ASP MET LEU CYS SER LYS VAL THR GLU THR GLU GLU GLU GLU ASP TYR ASN SER VAL ILE PRO THR SER MET VAL HIS GLY ARG LEU GLY PHE ASP GLY GLN TYR HIS GLU LYS ASP LEU
ASP VAL THR THR LEU PHE GLY ASP TRP VAL ALA ASN TYR PRO GLY VAL GLY GLY SER PHE ILE ASP ASN ARG VAL TRP PHE PRO VAL TYR GLY GLY LEU LYS PRO SER SER PRO SER ASP THR ALA GLN GLU GLY ARG TYR VAL ILE TYR LYS ARG TYR ASN ASP THR CYS PRO ASP
GLU GLN ASP TYR GLN ILE ARG MET ALA LYS SER SER TYR LYS PRO GLY ARG PHE GLY GLY LYS ARG VAL GLN GLN ALA ILE LEU SER ILE LYS VAL SER THR SER LEU GLY GLU ASP PRO VAL LEU THR ILE PRO PRO ASN THR VAL THR LEU MET GLY ALA GLU GLY ARG VAL LEU THR
VAL GLY THR SER HIS PHE LEU TYR GLN ARG GLY SER SER TYR PHE SER PRO ALA LEU LEU TYR PRO MET THR VAL ASN ASN ASN THR ALA THR LEU HIS SER PRO TYR THR PHE ASN ALA PHE THR ARG PRO GLY SER VAL PRO CYS GLN ALA SER ALA ARG CYS PRO ASN SER CYS VAL
THR GLY VAL TYR THR ASP PRO TYR PRO LEU VAL PHE HIS ARG ASN HIS THR LEU ARG GLY VAL PHE GLY THR MET LEU ASP ASP GLU GLN ALA ARG LEU ASN LEU VAL SER ALA VAL PHE ASP ASN ILE SER ARG SER ARG ILE THR ARG VAL SER SER SER ARG THR LYS ALA ALA TYR
THR THR SER THR CYS PHE LYS VAL VAL LYS THR ASN LYS THR TYR CYS LEU SER ILE ALA GLU ILE SER ASN THR LEU PHE GLY GLU PHE ARG ILE ILE VAL PRO LEU LEU VAL GLU ILE LEU LYS ASP ASP GLY VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	138.29Å 138.29Å 167.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.89 – 3.30 48.89 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.89-3.30) 100.0 (48.89-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.63 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.248 , 0.310 0.239 , 0.305	Depositor DCC
R_{free} test set	1240 reflections (4.96%)	DCC
Wilson B-factor (Å^2)	126.9	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 117.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 25027 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6976	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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	0.30	0/3288	0.52	0/4502
1	B	0.29	0/3278	0.51	0/4490
1	E	0.29	0/291	0.46	0/396
1	F	0.28	0/291	0.51	0/396
All	All	0.30	0/7148	0.51	0/9784

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	3204	0	2730	165	0
1	B	3194	0	2719	180	0
1	E	289	0	299	19	0
1	F	289	0	299	29	0
All	All	6976	0	6047	377	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 29.

All (377) 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:B:451:SER:H	1:B:466:THR:HG21	1.16	1.06
1:A:224:ARG:HG3	1:A:224:ARG:HH11	1.22	1.04
1:B:152:TYR:HE2	1:B:565:LEU:HB2	1.23	1.02
1:B:471:ASP:HB2	1:B:527:THR:HA	1.49	0.95
1:B:152:TYR:CE2	1:B:565:LEU:HB2	2.03	0.94
1:B:128:HIS:HD2	1:B:210:LEU:HB2	1.33	0.94
1:B:198:HIS:O	1:B:233:ASN:ND2	2.01	0.93
1:B:423:ALA:HB2	1:B:446:PHE:HD2	1.35	0.91
1:B:333:TYR:CE1	1:B:355:LYS:HA	2.06	0.90
1:A:158:GLU:HG2	1:B:168:THR:HG21	1.55	0.89
1:A:419:TYR:CD1	1:A:461:PRO:HA	2.08	0.88
1:A:224:ARG:CG	1:A:224:ARG:HH11	1.86	0.87
1:E:85:TYR:HE2	1:F:85:TYR:HB3	1.38	0.86
1:B:198:HIS:NE2	1:B:253:VAL:O	2.09	0.85
1:E:95:ALA:O	1:E:99:THR:HG23	1.77	0.85
1:B:353:MET:O	1:B:356:SER:N	2.10	0.84
1:B:347:GLN:N	1:B:347:GLN:OE1	2.12	0.82
1:F:79:ASP:OD2	1:F:80:VAL:HG23	1.79	0.82
1:E:82:ASP:OD1	1:E:83:ARG:N	2.11	0.82
1:B:198:HIS:CD2	1:B:198:HIS:C	2.54	0.81
1:B:128:HIS:HA	1:B:209:VAL:HG13	1.63	0.80
1:B:147:ASP:O	1:B:150:SER:OG	1.98	0.80
1:A:191:ILE:HG22	1:A:192:PHE:H	1.47	0.79
1:A:128:HIS:HA	1:A:209:VAL:HG13	1.65	0.78
1:B:261:TYR:HD2	1:B:363:PHE:HB3	1.50	0.77
1:A:167:THR:HG21	1:B:159:HIS:CD2	2.19	0.77
1:A:343:CYS:SG	1:A:350:GLN:NE2	2.58	0.76
1:A:329:GLN:HA	1:A:332:ARG:HD3	1.68	0.76
1:E:85:TYR:CE2	1:F:85:TYR:HB3	2.21	0.74
1:F:81:VAL:HG13	1:F:82:ASP:H	1.52	0.74
1:A:199:SER:O	1:A:233:ASN:ND2	2.20	0.74
1:B:126:PRO:O	1:B:127:VAL:HG13	1.89	0.73
1:F:80:VAL:HG22	1:F:83:ARG:HH22	1.54	0.72
1:E:85:TYR:OH	1:F:86:LYS:HA	1.89	0.72
1:B:349:TYR:CZ	1:B:353:MET:HE1	2.25	0.72
1:B:256:THR:N	1:B:259:GLU:OE2	2.16	0.71
1:A:522:LYS:HG3	1:A:548:SER:HB2	1.72	0.71
1:B:128:HIS:HA	1:B:209:VAL:CG1	2.20	0.70
1:B:423:ALA:HB2	1:B:446:PHE:CD2	2.24	0.70
1:A:503:ALA:HB2	1:A:513:ILE:HG22	1.72	0.70
1:A:282:GLU:HA	1:A:381:LEU:HD22	1.73	0.70
1:A:427:PRO:HG2	1:A:438:HIS:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:PRO:HD2	1:B:556:ARG:NH1	2.07	0.70
1:B:552:PHE:CD1	1:B:558:VAL:HG21	2.25	0.70
1:B:294:TRP:HA	1:B:319:LEU:HA	1.74	0.69
1:A:344:PRO:HD2	1:A:460:CYS:SG	2.33	0.69
1:A:533:VAL:HG22	1:A:536:THR:HG22	1.75	0.69
1:A:273:ARG:NH2	1:A:378:SER:O	2.25	0.69
1:B:148:VAL:HG23	1:B:484:ARG:NE	2.07	0.69
1:B:344:PRO:HD2	1:B:460:CYS:SG	2.34	0.68
1:B:503:ALA:HB2	1:B:513:ILE:HG22	1.74	0.68
1:A:192:PHE:HE2	1:B:158:GLU:HG2	1.58	0.68
1:A:224:ARG:HG3	1:A:224:ARG:NH1	1.97	0.68
1:A:563:GLU:HG2	1:A:565:LEU:HD21	1.74	0.68
1:B:310:ARG:HB2	1:B:312:TRP:NE1	2.09	0.67
1:A:158:GLU:CG	1:B:168:THR:HG21	2.23	0.67
1:A:552:PHE:O	1:B:556:ARG:NH2	2.24	0.67
1:B:198:HIS:HD2	1:B:198:HIS:C	1.97	0.67
1:B:511:SER:OG	1:B:512:ARG:O	2.13	0.67
1:A:267:THR:OG1	1:A:297:ASN:N	2.27	0.67
1:B:198:HIS:O	1:B:198:HIS:HD2	1.78	0.66
1:E:85:TYR:HE2	1:F:85:TYR:CB	2.07	0.66
1:B:148:VAL:HG21	1:B:484:ARG:HB3	1.77	0.66
1:A:473:TYR:CD1	1:A:529:THR:HA	2.30	0.66
1:B:146:SER:O	1:B:484:ARG:NH2	2.27	0.66
1:F:95:ALA:O	1:F:99:THR:HG23	1.97	0.65
1:A:425:LEU:HD11	1:A:472:PRO:HG2	1.77	0.65
1:A:191:ILE:HG22	1:A:192:PHE:N	2.10	0.65
1:B:388:THR:HG21	1:B:435:ALA:HB3	1.77	0.65
1:A:441:TYR:CE2	1:A:483:LEU:HB3	2.32	0.65
1:B:198:HIS:O	1:B:198:HIS:CD2	2.50	0.64
1:B:534:VAL:HG23	1:B:535:LYS:N	2.12	0.64
1:B:564:ILE:HD12	1:B:564:ILE:N	2.12	0.64
1:B:323:SER:H	1:B:326:ASP:HB3	1.62	0.64
1:A:522:LYS:CG	1:A:548:SER:HB2	2.28	0.64
1:A:417:SER:HA	1:A:466:THR:O	1.98	0.64
1:A:493:ASP:OD1	1:A:494:GLU:N	2.31	0.64
1:A:353:MET:SD	1:A:461:PRO:O	2.55	0.64
1:F:81:VAL:HG13	1:F:82:ASP:N	2.13	0.63
1:B:255:GLU:HB3	1:B:259:GLU:HG3	1.79	0.63
1:B:310:ARG:NH2	1:B:374:SER:O	2.32	0.63
1:B:548:SER:HA	1:B:554:GLU:O	1.98	0.63
1:A:247:ASP:OD1	1:A:273:ARG:HD3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASP:OD1	1:B:324:PRO:HD2	1.99	0.63
1:B:147:ASP:HA	1:B:484:ARG:HH22	1.63	0.62
1:A:446:PHE:CE1	1:A:490:MET:HB3	2.33	0.62
1:B:451:SER:H	1:B:466:THR:CG2	2.04	0.62
1:E:81:VAL:HA	1:E:84:ILE:HG22	1.80	0.62
1:F:109:SER:O	1:F:112:TYR:HB2	1.98	0.62
1:A:461:PRO:O	1:A:462:ASN:ND2	2.32	0.62
1:B:237:CYS:O	1:B:301:VAL:HA	1.99	0.62
1:A:148:VAL:HG23	1:A:484:ARG:CZ	2.28	0.62
1:A:192:PHE:HB2	1:A:200:HIS:NE2	2.14	0.62
1:F:114:ILE:O	1:F:114:ILE:HG13	1.99	0.62
1:B:487:PHE:HD1	1:B:503:ALA:O	1.83	0.61
1:B:261:TYR:HE1	1:B:296:ALA:HB3	1.66	0.61
1:A:242:THR:OG1	1:A:247:ASP:OD1	2.17	0.61
1:A:350:GLN:HG2	1:A:353:MET:HE3	1.82	0.61
1:B:446:PHE:CE1	1:B:490:MET:HB3	2.36	0.61
1:A:238:SER:HB2	1:A:302:GLY:O	2.01	0.61
1:B:491:LEU:HD11	1:B:523:ALA:HB3	1.83	0.61
1:A:345:ASP:HB2	1:A:350:GLN:HE21	1.65	0.60
1:B:406:VAL:HG21	1:B:474:PRO:HG2	1.83	0.60
1:B:233:ASN:O	1:B:252:LYS:HA	2.02	0.60
1:F:102:ILE:HD12	1:F:103:ILE:N	2.17	0.60
1:B:147:ASP:HA	1:B:484:ARG:NH2	2.17	0.60
1:A:168:THR:HG22	1:A:169:GLY:H	1.67	0.59
1:B:451:SER:N	1:B:466:THR:HG21	2.02	0.59
1:A:329:GLN:O	1:A:332:ARG:HG2	2.02	0.59
1:B:500:LEU:O	1:B:516:VAL:HG23	2.03	0.59
1:B:552:PHE:CE1	1:B:558:VAL:HG21	2.38	0.59
1:B:504:VAL:HG22	1:B:511:SER:HB3	1.85	0.59
1:B:131:ASP:O	1:B:534:VAL:HG22	2.03	0.58
1:A:174:ARG:HG2	1:A:546:GLU:CD	2.24	0.58
1:B:391:PRO:O	1:B:395:THR:HG22	2.03	0.58
1:B:128:HIS:CD2	1:B:210:LEU:HB2	2.25	0.58
1:A:306:PHE:CZ	1:A:309:ASN:HA	2.38	0.58
1:A:224:ARG:NH1	1:A:224:ARG:CG	2.57	0.58
1:E:92:SER:N	1:E:93:PRO:HD2	2.19	0.58
1:B:419:TYR:HA	1:B:454:CYS:SG	2.42	0.58
1:B:415:ARG:NE	1:B:417:SER:OG	2.37	0.57
1:B:242:THR:HB	1:B:243:PRO:HD2	1.86	0.57
1:A:455:GLN:OE1	1:A:455:GLN:N	2.31	0.57
1:B:349:TYR:O	1:B:353:MET:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PHE:HD1	1:A:200:HIS:HD2	1.52	0.57
1:B:541:CYS:SG	1:B:564:ILE:HD11	2.45	0.57
1:A:349:TYR:CD2	1:A:353:MET:HE1	2.40	0.57
1:A:267:THR:HG1	1:A:297:ASN:H	1.51	0.57
1:B:187:THR:HA	1:B:204:TYR:O	2.04	0.57
1:B:261:TYR:CD2	1:B:363:PHE:HB3	2.36	0.57
1:B:191:ILE:HG22	1:B:192:PHE:H	1.70	0.56
1:A:553:GLY:HA3	1:A:556:ARG:NH1	2.20	0.56
1:A:141:ILE:O	1:A:476:VAL:HA	2.06	0.56
1:A:350:GLN:HA	1:A:353:MET:HE2	1.88	0.56
1:A:526:THR:HA	1:A:544:ILE:O	2.06	0.56
1:B:273:ARG:HB3	1:B:381:LEU:HD21	1.87	0.56
1:B:444:ASN:C	1:B:446:PHE:H	2.09	0.56
1:F:80:VAL:O	1:F:80:VAL:HG12	2.05	0.56
1:A:234:ARG:HB3	1:A:250:CYS:HB3	1.86	0.55
1:E:91:GLU:O	1:E:94:LEU:HB2	2.06	0.55
1:B:471:ASP:CB	1:B:528:SER:H	2.18	0.55
1:A:498:LEU:HD23	1:A:522:LYS:HA	1.88	0.55
1:A:167:THR:O	1:A:167:THR:HG22	2.06	0.54
1:A:548:SER:HA	1:A:554:GLU:O	2.08	0.54
1:B:564:ILE:O	1:B:565:LEU:HD23	2.07	0.54
1:A:349:TYR:HD2	1:A:353:MET:CE	2.21	0.54
1:A:192:PHE:CE2	1:B:158:GLU:HG2	2.41	0.54
1:B:446:PHE:HD1	1:B:505:PHE:CZ	2.25	0.54
1:B:174:ARG:NH1	1:B:546:GLU:OE2	2.41	0.54
1:A:181:SER:OG	1:A:182:ALA:N	2.39	0.54
1:B:349:TYR:CE1	1:B:353:MET:HE1	2.43	0.54
1:A:349:TYR:CD2	1:A:353:MET:CE	2.91	0.54
1:B:271:HIS:CD2	1:B:382:GLY:H	2.26	0.54
1:A:187:THR:HA	1:A:204:TYR:O	2.08	0.54
1:B:419:TYR:CD2	1:B:461:PRO:HA	2.43	0.54
1:B:191:ILE:HG22	1:B:192:PHE:N	2.23	0.54
1:B:277:ASP:OD1	1:B:279:GLN:N	2.41	0.54
1:B:319:LEU:HD13	1:B:326:ASP:HB2	1.89	0.53
1:B:261:TYR:CE1	1:B:296:ALA:HB3	2.43	0.53
1:B:166:PRO:HD2	1:B:556:ARG:HH12	1.71	0.53
1:A:203:GLN:NE2	1:A:237:CYS:SG	2.80	0.53
1:E:109:SER:O	1:E:113:GLN:HG3	2.09	0.53
1:B:333:TYR:HE1	1:B:355:LYS:HA	1.71	0.53
1:A:142:VAL:O	1:A:142:VAL:HG23	2.07	0.53
1:A:162:PHE:CD1	1:A:220:PHE:HB2	2.45	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:HIS:CD2	1:B:210:LEU:H	2.27	0.52
1:A:339:TYR:H	1:A:444:ASN:ND2	2.08	0.52
1:B:423:ALA:HB3	1:B:443:PHE:HB2	1.92	0.52
1:F:82:ASP:OD1	1:F:83:ARG:HG3	2.09	0.52
1:A:184:HIS:CE1	1:A:222:THR:HG22	2.44	0.52
1:A:191:ILE:CG2	1:A:192:PHE:H	2.21	0.52
1:A:461:PRO:O	1:A:462:ASN:CG	2.47	0.52
1:F:113:GLN:O	1:F:114:ILE:C	2.48	0.52
1:A:506:ASP:OD1	1:A:507:ASN:N	2.40	0.51
1:A:478:HIS:HB3	1:A:480:ASN:HB2	1.91	0.51
1:A:144:ASP:OD1	1:A:479:ARG:HG2	2.10	0.51
1:A:350:GLN:HA	1:A:353:MET:CE	2.39	0.51
1:A:471:ASP:HB2	1:A:528:SER:H	1.76	0.51
1:B:238:SER:HB2	1:B:302:GLY:O	2.11	0.51
1:A:224:ARG:NE	1:A:276:PHE:O	2.41	0.51
1:F:81:VAL:CG1	1:F:82:ASP:H	2.20	0.51
1:B:561:LEU:HD12	1:B:562:VAL:H	1.75	0.51
1:A:256:THR:HG23	1:A:259:GLU:OE1	2.11	0.51
1:E:84:ILE:O	1:E:87:GLN:HG2	2.11	0.50
1:A:132:TYR:OH	1:A:218:VAL:HG22	2.11	0.50
1:F:80:VAL:HG13	1:F:83:ARG:HH12	1.76	0.50
1:A:396:LEU:HD22	1:A:419:TYR:HE2	1.77	0.50
1:B:480:ASN:O	1:B:481:HIS:HB2	2.12	0.50
1:B:411:PHE:CE1	1:B:441:TYR:HE2	2.28	0.50
1:B:152:TYR:CE2	1:B:565:LEU:HD12	2.47	0.50
1:A:339:TYR:H	1:A:444:ASN:HD21	1.60	0.50
1:A:397:MET:CE	1:A:465:VAL:HG22	2.42	0.50
1:B:132:TYR:OH	1:B:218:VAL:HG22	2.12	0.50
1:B:426:TYR:CD2	1:B:440:PRO:HB3	2.46	0.50
1:A:192:PHE:CD1	1:A:200:HIS:HD2	2.29	0.50
1:B:384:ASP:N	1:B:385:PRO:HD3	2.27	0.49
1:B:267:THR:HG23	1:B:296:ALA:HA	1.95	0.49
1:A:563:GLU:HG2	1:A:565:LEU:CD2	2.42	0.49
1:B:262:ASN:C	1:B:262:ASN:OD1	2.51	0.49
1:A:419:TYR:HD2	1:A:419:TYR:H	1.59	0.49
1:B:329:GLN:HA	1:B:329:GLN:OE1	2.13	0.49
1:A:188:HIS:CD2	1:A:188:HIS:C	2.85	0.49
1:A:479:ARG:C	1:A:481:HIS:H	2.15	0.49
1:A:300:GLY:C	1:A:302:GLY:H	2.16	0.49
1:E:86:LYS:HD3	1:E:86:LYS:O	2.13	0.49
1:B:392:ASN:HA	1:B:395:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:ASP:HB3	1:B:528:SER:H	1.78	0.49
1:F:83:ARG:HB3	1:F:86:LYS:HZ1	1.78	0.49
1:B:478:HIS:NE2	1:B:484:ARG:HG3	2.28	0.49
1:B:180:MET:HE1	1:B:220:PHE:HE2	1.78	0.48
1:B:333:TYR:O	1:B:393:THR:HA	2.13	0.48
1:B:256:THR:HG23	1:B:259:GLU:OE2	2.12	0.48
1:A:556:ARG:CZ	1:A:556:ARG:HB2	2.43	0.48
1:B:534:VAL:CG2	1:B:535:LYS:N	2.74	0.48
1:B:473:TYR:CD2	1:B:530:CYS:HB2	2.48	0.48
1:A:132:TYR:CE1	1:A:210:LEU:HD22	2.47	0.48
1:A:501:VAL:HG12	1:A:515:ARG:HG2	1.95	0.48
1:E:90:LEU:O	1:E:94:LEU:HD13	2.14	0.48
1:A:158:GLU:CD	1:B:168:THR:HG21	2.34	0.48
1:A:341:ASP:CB	1:A:459:ARG:CZ	2.92	0.48
1:A:230:ASP:OD1	1:A:232:GLN:HB2	2.14	0.48
1:B:345:ASP:HB3	1:B:349:TYR:HD2	1.78	0.48
1:B:487:PHE:HB2	1:B:504:VAL:HG12	1.96	0.47
1:A:323:SER:H	1:A:326:ASP:HB3	1.79	0.47
1:B:174:ARG:HG2	1:B:546:GLU:OE2	2.14	0.47
1:B:255:GLU:HB3	1:B:259:GLU:CG	2.43	0.47
1:A:527:THR:HG22	1:A:544:ILE:HB	1.96	0.47
1:B:411:PHE:HE1	1:B:427:PRO:HG3	1.79	0.47
1:A:233:ASN:O	1:A:252:LYS:HA	2.14	0.47
1:A:231:THR:OG1	1:A:232:GLN:N	2.47	0.47
1:B:419:TYR:HB3	1:B:462:ASN:O	2.14	0.47
1:B:420:PHE:CZ	1:B:422:PRO:HB2	2.49	0.47
1:B:184:HIS:O	1:B:184:HIS:ND1	2.48	0.47
1:B:338:ARG:NH1	1:B:457:SER:HA	2.29	0.47
1:E:82:ASP:OD1	1:E:83:ARG:HG3	2.15	0.47
1:B:148:VAL:CG2	1:B:484:ARG:HB3	2.45	0.46
1:A:238:SER:CB	1:A:302:GLY:O	2.63	0.46
1:B:312:TRP:CE3	1:B:374:SER:HB3	2.49	0.46
1:F:113:GLN:C	1:F:113:GLN:CD	2.74	0.46
1:A:127:VAL:HG11	1:F:108:THR:HG23	1.97	0.46
1:B:388:THR:O	1:B:388:THR:HG23	2.16	0.46
1:A:568:ASP:OD1	1:A:568:ASP:N	2.47	0.46
1:A:479:ARG:C	1:A:481:HIS:N	2.67	0.46
1:A:191:ILE:CG2	1:A:192:PHE:N	2.79	0.46
1:A:255:GLU:HB3	1:A:259:GLU:OE1	2.15	0.46
1:B:129:ASP:HB3	1:B:130:PRO:HD2	1.98	0.46
1:A:517:SER:HB3	1:A:521:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:SER:O	1:A:327:THR:HG23	2.15	0.46
1:F:82:ASP:O	1:F:85:TYR:N	2.36	0.46
1:A:247:ASP:OD2	1:A:273:ARG:NH1	2.48	0.46
1:A:151:PHE:HA	1:A:565:LEU:O	2.16	0.46
1:B:188:HIS:C	1:B:188:HIS:ND1	2.69	0.46
1:B:257:GLU:O	1:B:260:ASP:N	2.49	0.46
1:A:536:THR:HG23	1:A:538:LYS:HG3	1.97	0.45
1:B:446:PHE:CD1	1:B:505:PHE:CE1	3.04	0.45
1:A:473:TYR:HB2	1:A:528:SER:O	2.16	0.45
1:A:156:PHE:HZ	1:A:502:SER:HG	1.64	0.45
1:A:478:HIS:HB3	1:A:480:ASN:H	1.82	0.45
1:B:213:SER:OG	1:B:217:ARG:HB2	2.17	0.45
1:B:272:GLY:HA2	1:B:381:LEU:HD22	1.98	0.45
1:A:178:PHE:HZ	1:A:180:MET:HE2	1.81	0.45
1:A:132:TYR:OH	1:A:211:ARG:O	2.31	0.45
1:B:396:LEU:HD12	1:B:396:LEU:N	2.31	0.45
1:B:405:THR:HG23	1:B:405:THR:O	2.17	0.45
1:F:83:ARG:O	1:F:86:LYS:HG3	2.17	0.44
1:A:341:ASP:CB	1:A:459:ARG:NE	2.80	0.44
1:B:470:THR:O	1:B:472:PRO:HD3	2.17	0.44
1:F:103:ILE:O	1:F:106:ALA:HB3	2.17	0.44
1:A:381:LEU:N	1:A:381:LEU:HD12	2.32	0.44
1:B:319:LEU:HD12	1:B:319:LEU:O	2.18	0.44
1:A:426:TYR:CD2	1:A:440:PRO:HB3	2.53	0.44
1:B:139:GLU:HB3	1:B:477:PHE:CD2	2.53	0.44
1:B:349:TYR:CE1	1:B:353:MET:CE	3.01	0.44
1:F:81:VAL:CG1	1:F:82:ASP:N	2.79	0.44
1:A:167:THR:HG21	1:B:159:HIS:NE2	2.32	0.44
1:A:168:THR:HG22	1:A:169:GLY:N	2.33	0.44
1:A:166:PRO:HG3	1:A:173:THR:HG23	1.98	0.44
1:B:128:HIS:HE1	1:B:182:ALA:C	2.21	0.44
1:B:446:PHE:CD1	1:B:490:MET:HB3	2.52	0.44
1:B:564:ILE:N	1:B:564:ILE:CD1	2.81	0.43
1:B:471:ASP:HB2	1:B:528:SER:H	1.83	0.43
1:A:197:ASP:CB	1:A:200:HIS:CE1	3.00	0.43
1:B:132:TYR:OH	1:B:211:ARG:O	2.36	0.43
1:A:421:SER:HB3	1:A:422:PRO:HD3	2.00	0.43
1:B:528:SER:HB2	1:B:543:SER:OG	2.19	0.43
1:B:273:ARG:NH2	1:B:378:SER:O	2.51	0.43
1:B:224:ARG:HD3	1:B:224:ARG:HA	1.84	0.43
1:B:198:HIS:CE1	1:B:253:VAL:O	2.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ASP:O	1:A:507:ASN:C	2.55	0.43
1:B:487:PHE:CE2	1:B:541:CYS:CB	3.01	0.43
1:A:553:GLY:HA3	1:A:556:ARG:HH12	1.83	0.43
1:B:210:LEU:HD21	1:B:220:PHE:CE2	2.54	0.43
1:E:79:ASP:C	1:E:81:VAL:H	2.21	0.43
1:A:490:MET:HG2	1:A:505:PHE:HZ	1.84	0.43
1:A:479:ARG:H	1:A:479:ARG:HG2	1.51	0.43
1:E:103:ILE:HD13	1:F:103:ILE:HG21	2.00	0.43
1:E:94:LEU:O	1:E:95:ALA:C	2.57	0.43
1:B:479:ARG:O	1:B:481:HIS:ND1	2.52	0.43
1:A:349:TYR:HD2	1:A:353:MET:HE1	1.79	0.43
1:A:333:TYR:CD2	1:A:333:TYR:N	2.87	0.43
1:A:561:LEU:HD12	1:A:562:VAL:H	1.84	0.43
1:A:144:ASP:OD2	1:A:478:HIS:ND1	2.45	0.43
1:A:429:THR:HG22	1:A:436:THR:OG1	2.18	0.43
1:B:517:SER:HB3	1:B:521:THR:OG1	2.19	0.43
1:B:146:SER:O	1:B:484:ARG:NH1	2.52	0.43
1:A:188:HIS:CD2	1:A:188:HIS:O	2.72	0.43
1:B:154:SER:O	1:B:514:THR:HG21	2.17	0.43
1:B:372:ILE:O	1:B:388:THR:HG22	2.19	0.42
1:B:255:GLU:HB3	1:B:259:GLU:CD	2.40	0.42
1:A:220:PHE:CZ	1:A:542:LEU:HD22	2.54	0.42
1:A:419:TYR:CD2	1:A:419:TYR:N	2.88	0.42
1:B:174:ARG:HG2	1:B:546:GLU:CD	2.39	0.42
1:B:277:ASP:OD1	1:B:278:GLY:N	2.52	0.42
1:A:207:LEU:HD23	1:A:208:GLY:N	2.35	0.42
1:A:311:VAL:O	1:A:374:SER:HA	2.20	0.42
1:A:349:TYR:CE2	1:A:353:MET:HE1	2.54	0.42
1:B:310:ARG:HB2	1:B:312:TRP:CE2	2.54	0.42
1:B:561:LEU:HD12	1:B:562:VAL:N	2.34	0.42
1:A:443:PHE:N	1:A:443:PHE:CD1	2.88	0.42
1:B:504:VAL:CG2	1:B:511:SER:HB3	2.49	0.42
1:A:346:GLU:O	1:A:349:TYR:HB3	2.18	0.42
1:A:474:PRO:HB3	1:A:483:LEU:HD11	2.01	0.42
1:A:425:LEU:HD11	1:A:472:PRO:CG	2.46	0.42
1:A:468:VAL:HG12	1:A:469:TYR:N	2.35	0.42
1:B:353:MET:C	1:B:355:LYS:N	2.70	0.42
1:A:346:GLU:H	1:A:346:GLU:HG3	1.41	0.42
1:B:314:PRO:HG3	1:B:401:GLY:O	2.20	0.42
1:A:420:PHE:HD2	1:A:424:LEU:HD11	1.85	0.42
1:A:197:ASP:CB	1:A:200:HIS:HE1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLN:OE1	1:A:391:PRO:HA	2.19	0.42
1:A:142:VAL:CG2	1:A:142:VAL:O	2.67	0.41
1:A:404:LEU:HD23	1:A:404:LEU:N	2.35	0.41
1:B:181:SER:OG	1:B:182:ALA:N	2.45	0.41
1:B:256:THR:O	1:B:259:GLU:HG2	2.20	0.41
1:A:338:ARG:NH2	1:A:444:ASN:O	2.53	0.41
1:F:81:VAL:O	1:F:84:ILE:HG13	2.20	0.41
1:B:177:SER:HB3	1:B:187:THR:HG22	2.02	0.41
1:A:127:VAL:CG1	1:F:108:THR:HG23	2.50	0.41
1:A:305:SER:HB2	1:A:403:VAL:O	2.19	0.41
1:F:80:VAL:HA	1:F:83:ARG:CZ	2.51	0.41
1:B:468:VAL:HG12	1:B:470:THR:HG23	2.02	0.41
1:B:526:THR:HA	1:B:544:ILE:O	2.21	0.41
1:A:242:THR:HG22	1:A:306:PHE:HB2	2.03	0.41
1:A:135:GLY:HA3	1:A:532:LYS:O	2.20	0.41
1:B:208:GLY:HA3	1:B:222:THR:HA	2.02	0.41
1:A:338:ARG:NH2	1:A:444:ASN:OD1	2.53	0.41
1:A:404:LEU:H	1:A:404:LEU:HD23	1.85	0.41
1:B:332:ARG:C	1:B:333:TYR:CD2	2.94	0.41
1:A:293:ASP:OD1	1:A:323:SER:HB2	2.20	0.41
1:B:290:LEU:HG	1:B:291:PHE:CD1	2.56	0.41
1:B:234:ARG:HA	1:B:251:SER:O	2.21	0.41
1:E:79:ASP:OD2	1:E:80:VAL:HG23	2.21	0.41
1:B:478:HIS:CD2	1:B:484:ARG:HG3	2.55	0.41
1:B:310:ARG:NH1	1:B:384:ASP:OD2	2.52	0.41
1:B:300:GLY:N	1:B:314:PRO:O	2.51	0.41
1:A:500:LEU:O	1:A:516:VAL:HG23	2.20	0.41
1:A:159:HIS:CE1	1:B:167:THR:HG21	2.56	0.41
1:F:81:VAL:O	1:F:84:ILE:CG1	2.69	0.41
1:A:173:THR:O	1:A:174:ARG:HG3	2.21	0.41
1:A:340:ASN:O	1:A:340:ASN:OD1	2.38	0.41
1:A:176:PRO:HB3	1:A:557:ILE:HD13	2.04	0.40
1:B:357:SER:O	1:B:360:PRO:HD3	2.20	0.40
1:B:128:HIS:CE1	1:B:182:ALA:C	2.95	0.40
1:A:192:PHE:HB2	1:A:200:HIS:CD2	2.56	0.40
1:A:527:THR:CG2	1:A:544:ILE:HB	2.51	0.40
1:B:271:HIS:NE2	1:B:381:LEU:HD23	2.36	0.40
1:A:180:MET:HE3	1:A:220:PHE:HE2	1.86	0.40
1:A:349:TYR:CD2	1:A:353:MET:HE2	2.56	0.40
1:E:85:TYR:C	1:E:87:GLN:N	2.74	0.40
1:B:187:THR:OG1	1:B:204:TYR:O	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:TYR:HD2	1:B:152:TYR:H	1.69	0.40
1:B:250:CYS:HA	1:B:299:PRO:HG2	2.04	0.40
1:A:310:ARG:HG2	1:A:376:LYS:HA	2.02	0.40
1:B:564:ILE:C	1:B:565:LEU:HD23	2.42	0.40
1:B:247:ASP:OD2	1:B:273:ARG:NH1	2.54	0.40
1:A:180:MET:CE	1:A:220:PHE:HE2	2.35	0.40
1:B:525:TYR:CD1	1:B:525:TYR:N	2.88	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	445/537 (83%)	413 (93%)	31 (7%)	1 (0%)	52 85
1	B	443/537 (82%)	406 (92%)	36 (8%)	1 (0%)	52 85
1	E	35/537 (6%)	29 (83%)	5 (14%)	1 (3%)	6 34
1	F	35/537 (6%)	28 (80%)	7 (20%)	0	100 100
All	All	958/2148 (45%)	876 (91%)	79 (8%)	3 (0%)	46 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	VAL
1	B	301	VAL
1	E	80	VAL

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	313/463 (68%)	288 (92%)	25 (8%)	15 49
1	B	313/463 (68%)	288 (92%)	25 (8%)	15 49
1	E	34/463 (7%)	28 (82%)	6 (18%)	2 10
1	F	34/463 (7%)	32 (94%)	2 (6%)	24 63
All	All	694/1852 (38%)	636 (92%)	58 (8%)	14 46

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	CYS
1	A	144	ASP
1	A	147	ASP
1	A	168	THR
1	A	184	HIS
1	A	210	LEU
1	A	221	SER
1	A	224	ARG
1	A	228	LEU
1	A	232	GLN
1	A	247	ASP
1	A	260	ASP
1	A	267	THR
1	A	286	ASP
1	A	346	GLU
1	A	353	MET
1	A	442	THR
1	A	446	PHE
1	A	479	ARG
1	A	502	SER
1	A	521	THR
1	A	533	VAL
1	A	556	ARG
1	A	567	ASP
1	A	568	ASP
1	B	152	TYR
1	B	167	THR
1	B	168	THR

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Mol	Chain	Res	Type
1	B	184	HIS
1	B	185	CYS
1	B	188	HIS
1	B	198	HIS
1	B	222	THR
1	B	224	ARG
1	B	260	ASP
1	B	290	LEU
1	B	316	TYR
1	B	342	THR
1	B	353	MET
1	B	381	LEU
1	B	442	THR
1	B	481	HIS
1	B	506	ASP
1	B	525	TYR
1	B	526	THR
1	B	539	THR
1	B	543	SER
1	B	556	ARG
1	B	562	VAL
1	B	565	LEU
1	E	81	VAL
1	E	84	ILE
1	E	90	LEU
1	E	99	THR
1	E	110	LEU
1	E	115	ASN
1	F	82	ASP
1	F	113	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	HIS
1	A	340	ASN
1	A	350	GLN
1	A	462	ASN
1	B	128	HIS
1	B	271	HIS

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	447/537 (83%)	0.10	5 (1%) 82 78	83, 111, 163, 215	0
1	B	445/537 (82%)	0.26	33 (7%) 17 14	83, 144, 200, 255	0
1	E	37/537 (6%)	0.05	0 100 100	100, 132, 177, 191	0
1	F	37/537 (6%)	-0.14	0 100 100	103, 133, 203, 212	0
All	All	966/2148 (44%)	0.17	38 (3%) 43 36	83, 129, 190, 255	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	GLY	4.7
1	A	485	GLY	3.7
1	B	274	LEU	3.6
1	B	383	GLU	3.4
1	B	345	ASP	3.2
1	B	461	PRO	3.1
1	B	462	ASN	3.1
1	B	348	ASP	3.1
1	A	419	TYR	3.0
1	B	419	TYR	3.0
1	B	485	GLY	2.9
1	B	346	GLU	2.8
1	B	465	VAL	2.7
1	B	245	GLY	2.7
1	B	329	GLN	2.6
1	B	344	PRO	2.6
1	B	349	TYR	2.5
1	B	458	ALA	2.4
1	B	446	PHE	2.4
1	B	426	TYR	2.3
1	B	528	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	331	GLY	2.3
1	B	319	LEU	2.3
1	B	207	LEU	2.2
1	B	505	PHE	2.2
1	B	565	LEU	2.2
1	B	381	LEU	2.2
1	A	450	GLY	2.1
1	B	163	ILE	2.1
1	A	348	ASP	2.1
1	B	285	LEU	2.1
1	B	424	LEU	2.1
1	A	350	GLN	2.0
1	B	556	ARG	2.0
1	B	243	PRO	2.0
1	B	333	TYR	2.0
1	B	332	ARG	2.0
1	B	242	THR	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.