



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:10 AM GMT

PDB ID : 3HFG
Title : Crystal Structure of Human 11-beta-hydroxysteroid-dehydrogenase Bound to an Sulfonyl-piperazine Inhibitor
Authors : Bard, J.; Svenson, K.
Deposited on : 2009-05-11
Resolution : 2.30 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 ⓘ 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

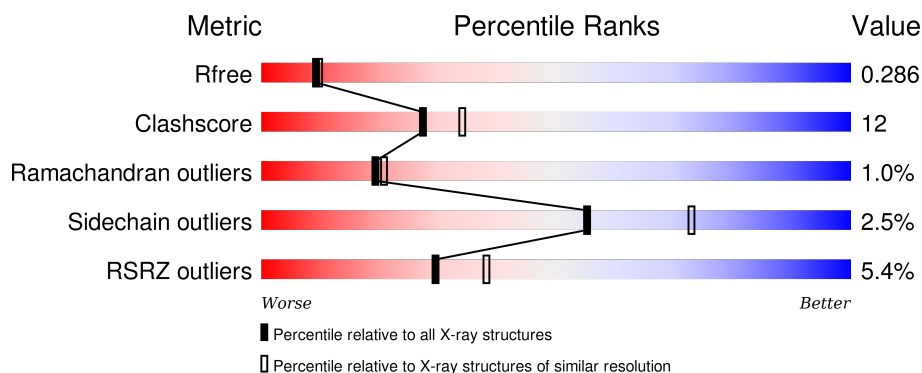
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	286	<div> <div>6%</div> <div>70%</div> <div>19%</div> <div>10%</div> </div>
1	B	286	<div> <div>3%</div> <div>72%</div> <div>19%</div> <div>9%</div> </div>
1	C	286	<div> <div>3%</div> <div>62%</div> <div>26%</div> <div>11%</div> </div>
1	D	286	<div> <div>7%</div> <div>57%</div> <div>30%</div> <div>11%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8217 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	1	0	0
			1959	1248	331	365	15			
1	B	260	Total	C	N	O	S	3	0	0
			1977	1260	335	367	15			
1	C	254	Total	C	N	O	S	3	0	0
			1914	1217	327	356	14			
1	D	254	Total	C	N	O	S	0	0	0
			1905	1209	326	356	14			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	EXPRESSION TAG	UNP P28845
A	8	LYS	-	EXPRESSION TAG	UNP P28845
A	9	HIS	-	EXPRESSION TAG	UNP P28845
A	10	GLN	-	EXPRESSION TAG	UNP P28845
A	11	HIS	-	EXPRESSION TAG	UNP P28845
A	12	GLN	-	EXPRESSION TAG	UNP P28845
A	13	HIS	-	EXPRESSION TAG	UNP P28845
A	14	GLN	-	EXPRESSION TAG	UNP P28845
A	15	HIS	-	EXPRESSION TAG	UNP P28845
A	16	GLN	-	EXPRESSION TAG	UNP P28845
A	17	HIS	-	EXPRESSION TAG	UNP P28845
A	18	GLN	-	EXPRESSION TAG	UNP P28845
A	19	HIS	-	EXPRESSION TAG	UNP P28845
A	20	GLN	-	EXPRESSION TAG	UNP P28845
A	21	GLN	-	EXPRESSION TAG	UNP P28845
A	22	PRO	-	EXPRESSION TAG	UNP P28845
A	23	LEU	-	EXPRESSION TAG	UNP P28845
A	272	SER	CYS	ENGINEERED	UNP P28845
B	7	MET	-	EXPRESSION TAG	UNP P28845
B	8	LYS	-	EXPRESSION TAG	UNP P28845
B	9	HIS	-	EXPRESSION TAG	UNP P28845

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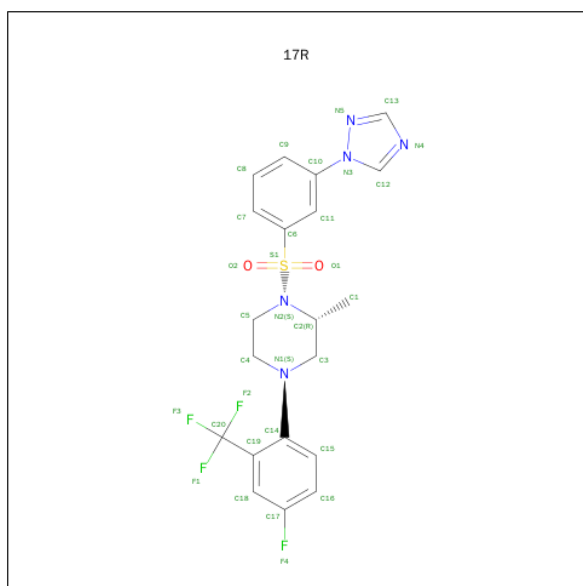
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	EXPRESSION TAG	UNP P28845
B	11	HIS	-	EXPRESSION TAG	UNP P28845
B	12	GLN	-	EXPRESSION TAG	UNP P28845
B	13	HIS	-	EXPRESSION TAG	UNP P28845
B	14	GLN	-	EXPRESSION TAG	UNP P28845
B	15	HIS	-	EXPRESSION TAG	UNP P28845
B	16	GLN	-	EXPRESSION TAG	UNP P28845
B	17	HIS	-	EXPRESSION TAG	UNP P28845
B	18	GLN	-	EXPRESSION TAG	UNP P28845
B	19	HIS	-	EXPRESSION TAG	UNP P28845
B	20	GLN	-	EXPRESSION TAG	UNP P28845
B	21	GLN	-	EXPRESSION TAG	UNP P28845
B	22	PRO	-	EXPRESSION TAG	UNP P28845
B	23	LEU	-	EXPRESSION TAG	UNP P28845
B	272	SER	CYS	ENGINEERED	UNP P28845
C	7	MET	-	EXPRESSION TAG	UNP P28845
C	8	LYS	-	EXPRESSION TAG	UNP P28845
C	9	HIS	-	EXPRESSION TAG	UNP P28845
C	10	GLN	-	EXPRESSION TAG	UNP P28845
C	11	HIS	-	EXPRESSION TAG	UNP P28845
C	12	GLN	-	EXPRESSION TAG	UNP P28845
C	13	HIS	-	EXPRESSION TAG	UNP P28845
C	14	GLN	-	EXPRESSION TAG	UNP P28845
C	15	HIS	-	EXPRESSION TAG	UNP P28845
C	16	GLN	-	EXPRESSION TAG	UNP P28845
C	17	HIS	-	EXPRESSION TAG	UNP P28845
C	18	GLN	-	EXPRESSION TAG	UNP P28845
C	19	HIS	-	EXPRESSION TAG	UNP P28845
C	20	GLN	-	EXPRESSION TAG	UNP P28845
C	21	GLN	-	EXPRESSION TAG	UNP P28845
C	22	PRO	-	EXPRESSION TAG	UNP P28845
C	23	LEU	-	EXPRESSION TAG	UNP P28845
C	272	SER	CYS	ENGINEERED	UNP P28845
D	7	MET	-	EXPRESSION TAG	UNP P28845
D	8	LYS	-	EXPRESSION TAG	UNP P28845
D	9	HIS	-	EXPRESSION TAG	UNP P28845
D	10	GLN	-	EXPRESSION TAG	UNP P28845
D	11	HIS	-	EXPRESSION TAG	UNP P28845
D	12	GLN	-	EXPRESSION TAG	UNP P28845
D	13	HIS	-	EXPRESSION TAG	UNP P28845
D	14	GLN	-	EXPRESSION TAG	UNP P28845
D	15	HIS	-	EXPRESSION TAG	UNP P28845

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Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	EXPRESSION TAG	UNP P28845
D	17	HIS	-	EXPRESSION TAG	UNP P28845
D	18	GLN	-	EXPRESSION TAG	UNP P28845
D	19	HIS	-	EXPRESSION TAG	UNP P28845
D	20	GLN	-	EXPRESSION TAG	UNP P28845
D	21	GLN	-	EXPRESSION TAG	UNP P28845
D	22	PRO	-	EXPRESSION TAG	UNP P28845
D	23	LEU	-	EXPRESSION TAG	UNP P28845
D	272	SER	CYS	ENGINEERED	UNP P28845

- Molecule 2 is (2R)-4-[4-FLUORO-2-(TRIFLUOROMETHYL)PHENYL]-2-METHYL-1-{{3-(1H-1,2,4-TRIAZOL-1-YL)PHENYL}SULFONYL}PIPERAZINE (three-letter code: 17R) (formula: C₂₀H₁₉F₄N₅O₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			32	20	4	5	2	1		
2	B	1	Total	C	F	N	O	S	0	0
			32	20	4	5	2	1		
2	C	1	Total	C	F	N	O	S	0	0
			32	20	4	5	2	1		
2	D	1	Total	C	F	N	O	S	0	0
			32	20	4	5	2	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).

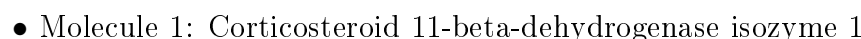
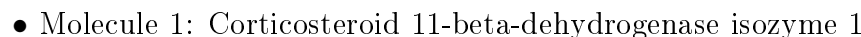


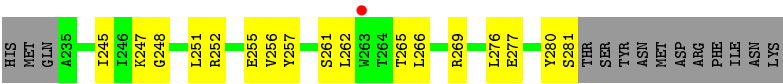
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

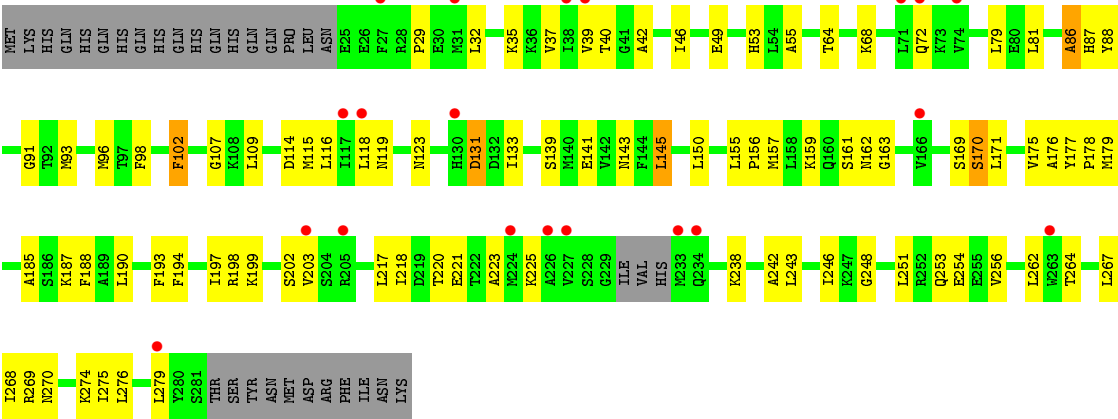
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	26	Total	O	0	0
			26	26		
4	C	52	Total	O	0	0
			52	52		
4	D	22	Total	O	0	0
			22	22		

- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1





● Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.44Å 152.67Å 74.20Å 90.00° 92.41° 90.00°	Depositor
Resolution (Å)	28.23 – 2.30 28.23 – 2.31	Depositor EDS
% Data completeness (in resolution range)	83.9 (28.23-2.30) 83.9 (28.23-2.31)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_6)	Depositor
R, R_{free}	0.231 , 0.285 0.229 , 0.286	Depositor DCC
R_{free} test set	2330 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.0	EDS
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 46179 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8217	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, 17R

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	0.28	0/1991	0.46	0/2689
1	B	0.26	0/2009	0.44	0/2711
1	C	0.28	0/1943	0.47	0/2622
1	D	0.27	0/1934	0.44	0/2612
All	All	0.27	0/7877	0.45	0/10634

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 [i](#)

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	1959	0	1993	39	0
1	B	1977	0	2014	40	0
1	C	1914	0	1941	57	0
1	D	1905	0	1917	67	0
2	A	32	0	19	1	0
2	B	32	0	19	2	0
2	C	32	0	19	3	0
2	D	32	0	19	1	0
3	A	48	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	25	4	0
3	C	48	0	25	3	0
3	D	48	0	25	6	0
4	A	42	0	0	1	0
4	B	26	0	0	1	0
4	C	52	0	0	2	0
4	D	22	0	0	0	0
All	All	8217	0	8041	191	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 (191) 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:D:39:VAL:HG12	1:D:42:ALA:HB2	1.61	0.83
1:A:233:MET:HG3	1:A:234:GLN:N	2.00	0.75
1:A:233:MET:HG3	1:A:234:GLN:H	1.52	0.74
1:A:133:ILE:HD13	1:B:149:VAL:HG22	1.71	0.72
1:C:171:LEU:HD12	2:C:1:17R:H7	1.72	0.72
1:D:223:ALA:HB2	3:D:293:NAP:H72N	1.55	0.71
1:C:39:VAL:HG12	1:C:42:ALA:HB2	1.74	0.69
1:B:64:THR:HB	1:B:102:PHE:CE1	2.29	0.68
1:B:91:GLY:HA3	1:B:98:PHE:CZ	2.29	0.67
1:D:46:ILE:HD11	1:D:218:ILE:HG13	1.75	0.66
1:A:93:MET:HG2	3:A:293:NAP:H2A	1.77	0.66
1:D:64:THR:HB	1:D:102:PHE:CE1	2.32	0.65
1:D:40:THR:HA	1:D:64:THR:HG22	1.78	0.65
1:D:141:GLU:HA	1:D:145:LEU:HB2	1.79	0.65
2:A:1:17R:H1	2:A:1:17R:C11	2.28	0.64
1:D:79:LEU:HD21	1:D:86:ALA:HB3	1.79	0.64
1:C:60:HIS:O	1:C:110:MET:HE2	1.99	0.63
1:C:134:HIS:HB2	4:C:324:HOH:O	1.99	0.63
1:C:180:VAL:O	1:C:180:VAL:HG23	1.99	0.63
1:D:91:GLY:HA3	1:D:98:PHE:CZ	2.35	0.62
1:D:139:SER:O	1:D:143:ASN:HB2	2.00	0.62
1:C:217:LEU:HD13	2:C:1:17R:H1B	1.83	0.61
1:C:261:SER:O	1:C:265:THR:HG23	2.01	0.61
1:B:39:VAL:HG12	1:B:42:ALA:HB2	1.82	0.61
2:B:1:17R:H1	2:B:1:17R:C11	2.33	0.59
1:C:193:PHE:HB2	1:D:185:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:LEU:HD22	1:D:150:LEU:HD12	1.84	0.58
1:C:60:HIS:C	1:C:110:MET:HE2	2.24	0.58
1:D:72:GLN:HG2	1:D:88:TYR:CE2	2.40	0.57
1:A:194:PHE:HA	1:A:197:ILE:HG12	1.86	0.57
1:D:68:LYS:O	1:D:72:GLN:HG3	2.04	0.56
1:A:199:LYS:HE3	1:A:277:GLU:HB3	1.86	0.56
1:C:194:PHE:CD2	1:C:197:ILE:HD11	2.40	0.56
1:D:171:LEU:HD21	1:D:268:ILE:HD11	1.88	0.56
1:A:215:LEU:HD11	1:A:245:ILE:HD11	1.87	0.55
1:D:32:LEU:HA	1:D:35:LYS:HG3	1.87	0.55
1:C:137:ARG:O	1:C:141:GLU:HG2	2.07	0.55
1:A:233:MET:CG	1:A:234:GLN:N	2.70	0.55
1:D:55:ALA:HB1	1:D:81:LEU:HB2	1.89	0.55
1:A:233:MET:CG	1:A:234:GLN:H	2.17	0.54
1:D:223:ALA:HB2	3:D:293:NAP:N7N	2.22	0.54
1:C:92:THR:OG1	1:C:94:GLU:HG3	2.07	0.54
1:A:185:ALA:HB2	1:B:193:PHE:HB2	1.89	0.54
1:A:48:ARG:NH2	1:A:73:LYS:HE3	2.23	0.54
1:B:40:THR:O	1:B:119:ASN:HB3	2.07	0.53
1:C:28:ARG:O	1:C:31:MET:HG3	2.08	0.53
1:C:93:MET:HG2	3:C:293:NAP:H2A	1.90	0.53
1:B:269:ARG:HH11	1:B:274:LYS:HE2	1.73	0.53
1:D:270:ASN:O	1:D:274:LYS:HG3	2.09	0.53
1:C:139:SER:O	1:C:143:ASN:HB2	2.10	0.52
1:D:187:LYS:HD2	1:D:190:LEU:HD12	1.90	0.52
1:D:107:GLY:HA3	1:D:157:MET:SD	2.50	0.52
1:D:40:THR:HA	1:D:64:THR:CG2	2.40	0.52
1:D:242:ALA:O	1:D:246:ILE:HG13	2.10	0.52
1:C:64:THR:HB	1:C:102:PHE:CE1	2.44	0.52
1:A:227:VAL:HG23	1:A:228:SER:N	2.25	0.51
1:C:43:SER:HB3	1:C:65:ALA:HB3	1.92	0.51
1:A:32:LEU:HA	1:A:35:LYS:HG3	1.92	0.51
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.93	0.51
1:D:248:GLY:HA3	1:D:256:VAL:HG21	1.91	0.51
1:A:155:LEU:HB3	1:A:156:PRO:HD3	1.92	0.50
1:B:66:ARG:HB2	3:B:293:NAP:O2X	2.11	0.50
1:C:280:TYR:O	1:C:281:SER:C	2.50	0.50
1:D:194:PHE:HA	1:D:197:ILE:HG12	1.94	0.50
1:D:49:GLU:HG3	1:D:238:LYS:HG3	1.93	0.50
1:B:170:SER:OG	3:B:293:NAP:H6N	2.11	0.49
1:C:26:GLU:HG2	1:C:27:PHE:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ASN:OD1	3:C:293:NAP:H4D	2.12	0.49
1:C:32:LEU:HD22	1:C:54:LEU:CD2	2.42	0.49
1:B:23:LEU:HD13	1:B:252:ARG:HD3	1.94	0.49
1:B:36:LYS:HB3	1:B:110:MET:HE3	1.95	0.49
1:C:257:TYR:CE1	1:C:269:ARG:HG2	2.48	0.49
1:B:93:MET:HG2	3:B:293:NAP:H2A	1.95	0.49
1:D:40:THR:HG22	1:D:64:THR:HG21	1.95	0.48
1:B:114:ASP:O	1:B:163:GLY:HA3	2.14	0.48
1:A:278:PHE:C	1:A:278:PHE:CD2	2.86	0.48
1:A:279:LEU:HD11	1:B:263:TRP:CH2	2.47	0.48
1:C:215:LEU:HD11	1:C:245:ILE:HD11	1.96	0.48
1:C:188:PHE:O	1:D:188:PHE:HB3	2.13	0.48
1:D:276:LEU:HA	1:D:279:LEU:HD12	1.96	0.48
1:C:230:ILE:C	1:C:230:ILE:HD13	2.34	0.47
1:C:194:PHE:HD2	1:C:197:ILE:HD11	1.79	0.47
1:D:264:THR:HA	1:D:267:LEU:HD12	1.96	0.47
1:D:175:VAL:CG2	1:D:177:TYR:CE1	2.97	0.47
1:B:233:MET:HE1	2:B:1:17R:H8	1.96	0.47
1:B:46:ILE:HG13	1:B:220:THR:HG21	1.97	0.47
1:D:170:SER:HB3	3:D:293:NAP:H5N	1.96	0.47
1:D:131:ASP:C	1:D:131:ASP:OD1	2.53	0.47
1:B:50:MET:O	1:B:54:LEU:HG	2.15	0.47
1:A:136:VAL:HG22	1:A:182:ALA:HB2	1.96	0.47
1:D:251:LEU:HB2	1:D:253:GLN:HG3	1.96	0.47
1:D:37:VAL:HG13	1:D:115:MET:HB3	1.97	0.46
1:D:178:PRO:O	1:D:179:MET:HB2	2.16	0.46
1:C:171:LEU:CD1	2:C:1:17R:H7	2.44	0.46
1:C:53:HIS:O	1:C:57:MET:HG3	2.15	0.46
1:C:63:VAL:HG23	1:C:71:LEU:HD22	1.97	0.46
1:C:178:PRO:O	1:C:179:MET:HB2	2.15	0.46
1:A:114:ASP:OD1	1:A:161:SER:HB2	2.16	0.46
1:B:134:HIS:HB2	4:B:308:HOH:O	2.16	0.46
1:C:27:PHE:CG	1:C:247:LYS:HG2	2.50	0.46
1:D:198:ARG:NH2	1:D:254:GLU:O	2.49	0.46
1:A:132:ASP:N	1:A:132:ASP:OD1	2.42	0.46
1:C:251:LEU:C	1:C:252:ARG:HG3	2.35	0.45
1:D:102:PHE:C	1:D:102:PHE:CD2	2.89	0.45
1:B:114:ASP:OD1	1:B:161:SER:HB2	2.15	0.45
1:B:35:LYS:HD3	1:B:35:LYS:HA	1.75	0.45
1:D:177:TYR:CD2	2:D:1:17R:N5	2.84	0.45
1:D:169:SER:O	3:D:293:NAP:H6N	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:O	1:A:266:LEU:HD13	2.15	0.45
1:B:236:ALA:HB1	1:B:258:TYR:HE1	1.81	0.45
1:B:105:GLN:O	1:B:109:LEU:HG	2.17	0.45
1:C:199:LYS:O	1:C:203:VAL:HG12	2.17	0.45
1:C:148:VAL:HG12	1:D:133:ILE:CD1	2.47	0.45
1:C:169:SER:O	3:C:293:NAP:H6N	2.17	0.45
1:C:178:PRO:O	1:C:179:MET:CB	2.64	0.45
1:B:244:GLU:HG3	1:B:258:TYR:CD2	2.51	0.45
1:D:161:SER:O	1:D:162:ASN:C	2.55	0.45
1:A:223:ALA:HB2	3:A:293:NAP:H72N	1.82	0.44
1:C:140:MET:HE2	1:C:140:MET:HA	1.99	0.44
1:B:170:SER:HB3	3:B:293:NAP:H5N	1.98	0.44
1:C:91:GLY:HA3	1:C:98:PHE:CZ	2.52	0.44
1:D:187:LYS:CD	1:D:190:LEU:HD12	2.48	0.44
1:C:43:SER:HB3	1:C:65:ALA:CB	2.48	0.44
1:C:88:TYR:CD1	1:C:88:TYR:C	2.90	0.44
1:D:93:MET:HG2	3:D:293:NAP:H2A	1.98	0.44
1:B:62:VAL:HG11	1:B:106:ALA:HB2	2.00	0.44
1:A:156:PRO:HD2	4:A:317:HOH:O	2.17	0.44
1:C:269:ARG:HB2	4:C:340:HOH:O	2.16	0.44
1:D:114:ASP:O	1:D:163:GLY:HA3	2.18	0.43
1:C:196:SER:O	1:C:200:GLU:HG3	2.18	0.43
1:B:201:TYR:CE2	1:B:210:ILE:HD11	2.53	0.43
1:A:29:PRO:HB3	1:A:57:MET:HG2	2.00	0.43
1:A:276:LEU:HA	1:A:276:LEU:HD12	1.85	0.43
1:B:200:GLU:HA	1:B:203:VAL:HG22	2.00	0.43
1:B:91:GLY:HA3	1:B:98:PHE:CE2	2.53	0.43
1:A:137:ARG:NH2	1:B:96:MET:HG3	2.33	0.43
1:D:116:LEU:HD11	1:D:118:LEU:HD21	2.00	0.43
1:B:39:VAL:CG1	1:B:42:ALA:HB2	2.47	0.43
1:C:94:GLU:HG2	1:C:142:VAL:CG2	2.49	0.42
1:B:263:TRP:HE3	1:D:275:ILE:HD13	1.84	0.42
1:D:217:LEU:O	1:D:218:ILE:HD13	2.19	0.42
1:B:263:TRP:HB2	1:D:275:ILE:HG12	2.01	0.42
1:D:53:HIS:CD2	1:D:243:LEU:HD13	2.54	0.42
1:C:262:LEU:O	1:C:266:LEU:HG	2.20	0.42
1:D:46:ILE:HG13	1:D:220:THR:HG21	2.01	0.42
1:C:212:LEU:O	1:C:255:GLU:HA	2.20	0.42
1:C:185:ALA:HB2	1:D:193:PHE:HB2	2.01	0.42
1:A:236:ALA:HB1	1:A:237:PRO:HD2	2.01	0.42
1:A:237:PRO:HG2	1:A:240:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:HB2	1:A:30:GLU:OE2	2.19	0.42
1:A:170:SER:HB3	3:A:293:NAP:H5N	2.01	0.42
1:A:236:ALA:HB1	1:A:258:TYR:CE1	2.55	0.42
1:C:194:PHE:HA	1:C:197:ILE:HG12	2.00	0.42
1:B:203:VAL:HG23	1:B:204:SER:N	2.34	0.42
1:A:77:HIS:O	1:A:81:LEU:HG	2.20	0.42
1:C:140:MET:HE2	1:C:186:SER:HB3	2.02	0.42
1:A:116:LEU:HG	1:A:118:LEU:HD21	2.02	0.42
1:D:269:ARG:NH1	1:D:274:LYS:NZ	2.67	0.42
1:A:281:SER:O	1:A:283:SER:N	2.53	0.42
1:B:46:ILE:HG13	1:B:220:THR:CG2	2.50	0.41
1:D:155:LEU:HB3	1:D:156:PRO:HD3	2.02	0.41
1:D:119:ASN:OD1	3:D:293:NAP:H4D	2.20	0.41
1:A:263:TRP:CD1	1:A:263:TRP:N	2.89	0.41
1:A:257:TYR:CD2	1:A:268:ILE:HG21	2.55	0.41
1:D:116:LEU:HD11	1:D:118:LEU:CD2	2.51	0.41
1:A:194:PHE:CD2	1:A:197:ILE:HD11	2.55	0.41
1:D:199:LYS:O	1:D:203:VAL:HG13	2.21	0.41
1:C:64:THR:HB	1:C:102:PHE:CZ	2.55	0.41
1:C:133:ILE:O	1:C:133:ILE:HG13	2.19	0.41
1:B:221:GLU:O	1:B:225:LYS:HG3	2.20	0.41
1:B:242:ALA:O	1:B:246:ILE:HG13	2.21	0.41
1:D:171:LEU:HA	1:D:171:LEU:HD23	1.97	0.41
1:A:279:LEU:HD11	1:B:263:TRP:CZ3	2.55	0.41
1:C:63:VAL:O	1:C:88:TYR:HA	2.21	0.41
1:D:87:HIS:ND1	1:D:109:LEU:HD23	2.36	0.41
1:B:269:ARG:HH11	1:B:274:LYS:CE	2.34	0.41
1:D:155:LEU:HG	1:D:159:LYS:HE3	2.02	0.41
1:C:276:LEU:HD21	1:D:267:LEU:HB2	2.03	0.40
1:C:152:VAL:HG21	1:D:133:ILE:HD11	2.02	0.40
1:A:248:GLY:HA3	1:A:256:VAL:HG21	2.03	0.40
1:C:64:THR:O	1:C:65:ALA:HB2	2.21	0.40
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.96	0.40
1:B:171:LEU:HD21	1:B:268:ILE:HD11	2.01	0.40
1:D:145:LEU:HD13	1:D:145:LEU:HA	1.78	0.40
1:A:155:LEU:HG	1:A:159:LYS:HE3	2.04	0.40
1:D:221:GLU:OE2	1:D:225:LYS:HD2	2.21	0.40
1:D:93:MET:O	1:D:96:MET:CE	2.69	0.40
1:D:91:GLY:HA3	1:D:98:PHE:CE2	2.56	0.40
1:D:88:TYR:CD1	1:D:88:TYR:C	2.94	0.40
1:C:277:GLU:HG2	1:D:176:ALA:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:VAL:O	1:C:187:LYS:NZ	2.53	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	256/286 (90%)	240 (94%)	12 (5%)	4 (2%)	12	11
1	B	256/286 (90%)	236 (92%)	19 (7%)	1 (0%)	39	48
1	C	250/286 (87%)	234 (94%)	14 (6%)	2 (1%)	24	27
1	D	250/286 (87%)	227 (91%)	20 (8%)	3 (1%)	16	16
All	All	1012/1144 (88%)	937 (93%)	65 (6%)	10 (1%)	19	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	ILE
1	C	65	ALA
1	A	65	ALA
1	A	282	THR
1	B	65	ALA
1	D	86	ALA
1	A	228	SER
1	C	68	LYS
1	D	262	LEU
1	D	29	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	211/243 (87%)	206 (98%)	5 (2%)	57	74
1	B	213/243 (88%)	208 (98%)	5 (2%)	58	75
1	C	203/243 (84%)	198 (98%)	5 (2%)	55	73
1	D	201/243 (83%)	195 (97%)	6 (3%)	48	65
All	All	828/972 (85%)	807 (98%)	21 (2%)	55	73

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	LEU
1	A	170	SER
1	A	221	GLU
1	A	276	LEU
1	A	279	LEU
1	B	76	SER
1	B	145	LEU
1	B	170	SER
1	B	184	SER
1	B	234	GLN
1	C	30	GLU
1	C	145	LEU
1	C	170	SER
1	C	203	VAL
1	C	230	ILE
1	D	102	PHE
1	D	123	ASN
1	D	131	ASP
1	D	145	LEU
1	D	170	SER
1	D	202	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	17R	A	1	-	30,35,35	1.16	1 (3%)	45,53,53	1.35	7 (15%)
3	NAP	A	293	-	42,52,52	1.08	2 (4%)	54,80,80	1.94	9 (16%)
2	17R	B	1	-	30,35,35	1.33	1 (3%)	45,53,53	1.33	7 (15%)
3	NAP	B	293	-	42,52,52	1.08	3 (7%)	54,80,80	1.85	7 (12%)
2	17R	C	1	-	30,35,35	1.29	1 (3%)	45,53,53	1.53	4 (8%)
3	NAP	C	293	-	42,52,52	1.08	2 (4%)	54,80,80	1.97	9 (16%)
2	17R	D	1	-	30,35,35	1.29	1 (3%)	45,53,53	1.56	5 (11%)
3	NAP	D	293	-	42,52,52	1.13	2 (4%)	54,80,80	1.98	7 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	17R	A	1	-	-	0/26/39/39	0/4/4/4
3	NAP	A	293	-	-	0/27/67/67	0/5/5/5
2	17R	B	1	-	-	0/26/39/39	0/4/4/4
3	NAP	B	293	-	-	0/27/67/67	0/5/5/5
2	17R	C	1	-	-	0/26/39/39	0/4/4/4
3	NAP	C	293	-	-	0/27/67/67	0/5/5/5
2	17R	D	1	-	-	0/26/39/39	0/4/4/4
3	NAP	D	293	-	-	0/27/67/67	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	293	NAP	C8A-N7A	-2.30	1.30	1.34
3	B	293	NAP	O4D-C1D	2.63	1.44	1.41
3	A	293	NAP	O4B-C1B	2.65	1.44	1.41
3	B	293	NAP	O4B-C1B	2.81	1.44	1.41
3	C	293	NAP	O4D-C1D	2.97	1.45	1.41
3	C	293	NAP	O4B-C1B	3.02	1.45	1.41
3	A	293	NAP	O4D-C1D	3.04	1.45	1.41
3	D	293	NAP	O4B-C1B	3.08	1.45	1.41
3	D	293	NAP	O4D-C1D	3.22	1.45	1.41
2	A	1	17R	S1-N2	4.19	1.69	1.63
2	C	1	17R	S1-N2	4.44	1.69	1.63
2	D	1	17R	S1-N2	4.95	1.70	1.63
2	B	1	17R	S1-N2	5.39	1.71	1.63

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	293	NAP	N3A-C2A-N1A	-8.45	122.42	128.89
3	D	293	NAP	N3A-C2A-N1A	-8.43	122.44	128.89
3	B	293	NAP	N3A-C2A-N1A	-8.41	122.45	128.89
3	C	293	NAP	N3A-C2A-N1A	-8.37	122.49	128.89
3	C	293	NAP	PN-O3-PA	-8.10	109.99	132.73
3	D	293	NAP	PN-O3-PA	-7.65	111.26	132.73
3	B	293	NAP	PN-O3-PA	-6.75	113.78	132.73
3	A	293	NAP	PN-O3-PA	-6.32	114.98	132.73
2	D	1	17R	C6-S1-N2	-5.98	97.60	107.38
2	C	1	17R	C6-S1-N2	-5.77	97.96	107.38
3	D	293	NAP	P2B-O2B-C2B	-4.97	109.63	121.56
3	B	293	NAP	P2B-O2B-C2B	-3.51	113.14	121.56
2	A	1	17R	C20-C19-C14	-3.14	117.83	122.07
3	B	293	NAP	C4A-C5A-N7A	-2.94	106.77	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	17R	C9-C10-C11	-2.78	118.98	121.50
2	D	1	17R	C3-N1-C14	-2.77	112.19	120.27
3	C	293	NAP	P2B-O2B-C2B	-2.65	115.22	121.56
2	B	1	17R	C5-N2-C2	-2.54	112.73	116.38
2	A	1	17R	C6-S1-N2	-2.52	103.27	107.38
3	A	293	NAP	P2B-O2B-C2B	-2.48	115.61	121.56
3	A	293	NAP	C4A-C5A-N7A	-2.45	107.23	109.48
3	D	293	NAP	C4A-C5A-N7A	-2.43	107.24	109.48
3	C	293	NAP	C4A-C5A-N7A	-2.41	107.27	109.48
3	D	293	NAP	C4B-O4B-C1B	-2.25	107.25	109.72
2	B	1	17R	C7-C6-S1	-2.23	117.33	119.79
2	B	1	17R	C20-C19-C14	-2.20	119.09	122.07
3	B	293	NAP	O7N-C7N-N7N	-2.15	119.57	122.59
3	C	293	NAP	C3B-C2B-C1B	-2.14	98.59	102.73
3	A	293	NAP	O7N-C7N-N7N	-2.10	119.64	122.59
3	C	293	NAP	C5B-C4B-C3B	-2.06	107.03	115.21
3	C	293	NAP	O2B-C2B-C3B	-2.05	103.55	111.51
2	A	1	17R	C12-N3-C10	2.00	130.17	126.02
3	C	293	NAP	O3-PA-O5B	2.06	108.39	102.94
2	A	1	17R	C4-N1-C3	2.11	117.73	113.30
3	C	293	NAP	O4D-C1D-N1N	2.15	110.50	108.13
2	B	1	17R	C11-C10-N3	2.19	121.80	119.13
2	D	1	17R	C4-C5-N2	2.21	111.03	109.07
3	B	293	NAP	O2B-P2B-O1X	2.22	112.66	107.11
2	B	1	17R	C18-C19-C20	2.23	121.48	116.51
2	C	1	17R	C18-C19-C20	2.24	121.49	116.51
3	D	293	NAP	O3-PA-O5B	2.27	108.95	102.94
3	A	293	NAP	O3-PA-O5B	2.42	109.37	102.94
3	A	293	NAP	O2B-P2B-O1X	2.43	113.18	107.11
3	D	293	NAP	O3-PN-O5D	2.43	109.39	102.94
3	B	293	NAP	C3N-C7N-N7N	2.44	120.48	117.82
2	A	1	17R	C18-C19-C20	2.59	122.28	116.51
2	B	1	17R	C4-N1-C3	2.63	118.81	113.30
2	A	1	17R	C2-N2-S1	2.76	125.81	119.88
2	C	1	17R	C4-C5-N2	2.85	111.60	109.07
2	A	1	17R	C10-N3-N5	3.15	121.67	118.89
3	A	293	NAP	C3N-C7N-N7N	3.23	121.35	117.82
2	B	1	17R	C10-N3-N5	3.29	121.80	118.89
2	C	1	17R	C10-N3-N5	4.03	122.45	118.89
3	A	293	NAP	O4D-C1D-N1N	4.11	112.65	108.13
2	D	1	17R	C10-N3-N5	4.15	122.55	118.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	17R	1	0
3	A	293	NAP	3	0
2	B	1	17R	2	0
3	B	293	NAP	4	0
2	C	1	17R	3	0
3	C	293	NAP	3	0
2	D	1	17R	1	0
3	D	293	NAP	6	0

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	258/286 (90%)	0.19	17 (6%)	22 29	34, 50, 80, 98	2 (0%)
1	B	260/286 (90%)	0.11	9 (3%)	48 56	36, 54, 75, 97	4 (1%)
1	C	254/286 (88%)	0.12	9 (3%)	48 56	32, 49, 76, 90	3 (1%)
1	D	254/286 (88%)	0.46	20 (7%)	15 22	36, 62, 85, 94	4 (1%)
All	All	1026/1144 (89%)	0.22	55 (5%)	29 38	32, 53, 82, 98	13 (1%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263	TRP	5.6
1	C	263	TRP	4.9
1	D	226	ALA	4.4
1	D	263	TRP	4.3
1	C	228	SER	4.2
1	D	39	VAL	4.1
1	A	229	GLY	4.0
1	D	27	PHE	3.8
1	D	117	ILE	3.7
1	C	126	LEU	3.7
1	D	224	MET	3.6
1	D	166	VAL	3.3
1	D	205	ARG	3.3
1	C	227	VAL	3.2
1	A	231	VAL	3.2
1	C	229	GLY	3.1
1	A	228	SER	3.0
1	B	24	ASN	2.9
1	A	167	VAL	2.8
1	D	72	GLN	2.8
1	A	118	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	166	VAL	2.7
1	B	262	LEU	2.6
1	B	81	LEU	2.6
1	C	24	ASN	2.6
1	D	279	LEU	2.6
1	A	202	SER	2.6
1	B	23	LEU	2.6
1	A	233	MET	2.5
1	A	205	ARG	2.5
1	B	167	VAL	2.4
1	C	167	VAL	2.4
1	D	31	MET	2.4
1	D	203	VAL	2.3
1	A	281	SER	2.3
1	A	168	VAL	2.3
1	D	71	LEU	2.3
1	D	118	LEU	2.3
1	B	234	GLN	2.2
1	D	233	MET	2.2
1	D	227	VAL	2.2
1	D	74	VAL	2.2
1	A	189	ALA	2.2
1	B	263	TRP	2.1
1	B	25	GLU	2.1
1	A	282	THR	2.1
1	A	230	ILE	2.1
1	C	27	PHE	2.1
1	C	205	ARG	2.1
1	D	130	HIS	2.1
1	A	266	LEU	2.1
1	D	234	GLN	2.1
1	A	262	LEU	2.0
1	D	38	ILE	2.0
1	B	190	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	17R	C	1	32/32	0.93	0.19	0.42	38,58,71,73	0
2	17R	D	1	32/32	0.94	0.17	-0.08	55,62,71,74	0
3	NAP	C	293	48/48	0.95	0.13	-0.16	35,42,51,60	0
2	17R	A	1	32/32	0.95	0.13	-0.25	42,51,61,66	0
3	NAP	A	293	48/48	0.95	0.11	-0.57	34,42,50,55	0
2	17R	B	1	32/32	0.96	0.12	-0.73	48,57,65,69	0
3	NAP	B	293	48/48	0.96	0.11	-0.73	37,47,56,61	0
3	NAP	D	293	48/48	0.95	0.10	-1.41	47,57,69,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.